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On Wiener Index and Variants of Szeged Index of Single Walled Titania Nanotubes $TiO_2(m, n)^*$

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Abstract. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. There are certain types of topological indices such as degree based topological indices, distance based topological indices and counting related topological indices etc. These topological indices correlate certain physico-chemical properties such as boiling point, stability and strain energy etc. of chemical compounds.

In this paper we compute an exact expression of Wiener index, vertex-Szeged index, edge-Szeged index and total-Szeged Index of single walled titania nanotubes $TiO_2(m, n)$ by using the cut-method for all values of m and n .

Keywords: Wiener index, Vertex-Szeged index, Edge-Szeged Index, Total-Szeged index, $TiO_2(m, n)$ nanotube.

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1 Introduction and preliminary results

The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in QSAR/QSPR study. In the last few years, the number of proposed molecular descriptors is rapidly increasing. Topological indices play a vital role in QSAR/QSPR study [1]. They correlate the certain physico-chemical properties of chemical compounds. Randić index has been closely correlated with many chemical properties and found to parallel the boiling point and Kovats constants [2]. The atom-bond connectivity (ABC) index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. For certain physico-chemical properties, the predictive power of connectivity topological descriptor known as *geometric – arithmetic* (GA) index is somewhat better than predictive power of the Randić connectivity index. Graph theory has provided chemist with a variety of useful tools, such as topological indices. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. *Cheminformatics* is a new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR/QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index and *ABC* index are used to predict bioactivity of the chemical compounds [3].

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix. A *topological index* is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. In a more precise way, a *topological index* $Top(G)$ of a graph, is a number with the property that for every graph H isomorphic to G , $Top(H) = Top(G)$. The concept of topological indices came from Wiener [4] while he was working on boiling point of paraffin, named this index as *path number*. Later on, the path number was renamed as *Wiener index* [5]. A molecular descriptor is a numeric number which represents the whole structure of a chemical graph. They have been found many application in quantitative structure-activity (QSAR) and structure-property relationship (QSPR) study. There is a basic difference between a molecular and topological descriptors that a molecular descriptor is just a representation of underlying chemical structure but a topological index/descriptors correlate certain physico-chemical properties of underlying chemical structure in addition to

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represent the whole structure. Due to this correlation property, topological indices found diverse applications in nanobiotechnology and QSAR/QSPR study.

In this article, G is considered to be a molecular network with vertex set $V(G)$ and edge set $E(G)$, $\deg(u)$ is the degree of vertex $u \in V(G)$. The notations used in this article are mainly taken from books [6–8].

Let G be a connected graph. Then the *Wiener index* of G is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u,v) \quad (1)$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic.

In theoretical computer science, Wiener index is considered as one of basic descriptors of fixed interconnection network because it provides the average distance between any two nodes of the network. The Szeged index was introduced by Gutman and it was closely related to Wiener index. It is well known that for trees the Wiener and Szeged indices are equal. Many physico-chemical properties related to organic compounds acting as drugs were modeled by using Szeged index.

The vertex-Szeged index [9] of the graph G is defined as

$$Sz_v(G) = \sum_{e \in E(G)} n_u(e) \times n_v(e).$$

The edge-Szeged index [10] of the graph G is defined as

$$Sz_e(G) = \sum_{e \in E(G)} m_u(e) \times m_v(e).$$

where $n_u(e)(m_u(e))$ is the number of vertices(edges) whose distance to the vertex u is smaller than the distance to the vertex v and $n_v(e)(m_v(e))$ is the number of vertices(edges) whose distance to the vertex v is smaller than the distance to the vertex u .

The edge-vertex-Szeged index [10] of a graph G is defined as

$$Sz_e(G) = \frac{1}{2} \sum_{e \in E(G)} n_u(e) \times m_v(e) + n_v(e) \times m_u(e).$$

The total-Szeged index [11] of the graph G is defined as

$$Sz_t(G) = \sum_{e \in E(G)} t_u(e) \times t_v(e).$$

where $t_u(e)$ is the number of vertices and edges of G whose distance to vertex u is smaller than the distance to vertex v and $t_v(e)$ is defined analogously.

Hence

$$Sz_t(G) = \sum_{e \in E(G)} \{n_u(e) + m_u(e)\} \times \{n_v(e) + m_v(e)\}.$$

Therefore

$$Sz_t(G) = Sz_v(G) + Sz_e(G) + 2Sz_v(G).$$

Let G be a connected graph. Then $e = (x, y)$ and $f = (u, v)$ are in the *Djokovic-Winkler relation* Θ if $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$. The relation Θ is always reflexive and symmetric, and transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes $F_1, F_2, \dots, F_k$, called Θ -classes or cuts. The cut method was introduced in [12] and used to compute the Wiener index of graphs which admit isometric embeddings into hypercubes. The result was extended to general graphs by establishing a connection between the Wiener index of a graph and its canonical metric representation [13]. The same method was successively applied to vertex-Szeged index, edge-Szeged index and total-Szeged index. For recent updates on cut method, we encourage the readers to [14].

Theorem 1.0.1. [14] Let G be a partial cube and let $F_1, F_2, \dots, F_k$ be its Θ -classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Let $m_1(F_i)$ and $m_2(F_i)$ be the number of edges in the two connected components of GF_i . Let $t_1(F_i)$ and $t_2(F_i)$ be the number of vertices and edges in the two connected components of $G - F_i$. Then

$$W(G) = \sum_{i=1}^k n_1(F_i) \times n_2(F_i)$$

$$Sz_v(G) = \sum_{i=1}^k |F_i| \{n_1(F_i) \times n_2(F_i)\}$$

$$Sz_e(G) = \sum_{i=1}^k |F_i| \{m_1(F_i) \times m_2(F_i)\}$$

$$Sz_{ev}(G) = \frac{1}{2} \sum_{i=1}^k |F_i| \{n_1(F_i) \times m_2(F_i) + n_2(F_i) \times m_1(F_i)\}$$

$$Sz_t(G) = \sum_{i=1}^k |F_i| \{t_1(F_i) \times t_2(F_i)\}$$

In this paper, we compute the Wiener index, vertex-Szeged index, edge-Szeged index, edge-vertex-Szeged index and total-Szeged index of $TiO_2(m, n)$ nanotubes using cut method. For recent results on different topological indices of nanotubes, we refer the readers to consult [3, 15–26]. For Szeged index of carbon nanotubes, please consult [24, 25, 27].

2 Main results on Wiener index and Szeged index of $TiO_2(m, n)$ nanotubes

As a well-known semiconductor with numerous technological applications, titania nanotubes were comprehensively studied in materials science. Titania nanotubes were systematically synthesized during the last 10-15 years using different methods and carefully studied as prospective technological materials. Since the growth mechanism for TiO_2 nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable. The $TiO_2(m, n)$ nanotubes were parameterized in [28].

The graph of the titania nanotube $TiO_2(m, n)$ is presented in Fig. 1, where m denotes the number of octagons in a column and n denotes the number of octagons in a row of the titania nanotube. The vertex and edge

Fig. 1. $TiO_2(m, n)$ nanotube

counts of $TiO_2(m, n)$ graph are respectively given by $|V(G)| = 12mn$ and $|E(G)| = 20mn - 4m - 2n$. In this section, we compute the Wiener index and the different variants of Szeged index of $TiO_2(m, n)$ nanotubes. For computation purpose, we have used the Maple software.

Theorem 2.0.1. For every positive integer $m > n$, the exact expressions for the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:

$$\bullet W(TiO_2(m, n)) = -164 + \frac{4112}{15}n + 192m^3n^2 + \frac{20}{3}n^3 - \frac{24}{5}n^5 + 24n^4m - 112n^2 - 20mn^2 + 112mn - 164m.$$

$$\bullet Sz_v(TiO_2(m, n)) = 328 - \frac{18092}{15}n + 480m^3n^3 - 96m^3n^2 - \frac{96}{5}n^5 + 48n^4m + 464n^2m - \frac{1352}{3}n^3 - 880mn - 56mn^3 + 28n^4 + 1320n^2 + 328m.$$

$$\bullet Sz_e(TiO_2(m, n)) = \frac{82}{3}n - \frac{2240}{3}m^3n^2 + 672m^2n^2 + \frac{416}{3}m^3n + \frac{4000}{3}m^3n^3 - 176n^5 - 960m^2n^3 - 184m^2n - \frac{32}{3}m^3 + 16m^2 + 236n^4 + \frac{2000}{3}n^4m + \frac{152}{3}n^3 - \frac{3056}{3}mn^3 + 412mn^2 - 138n^2 - \frac{64}{3}mn - \frac{16}{3}m.$$

$$\bullet Sz_{ev}(TiO_2(m, n)) = 36 - \frac{4711}{30}n + 284mn + 960m^3n^3 - 352m^3n^2 - \frac{1334}{3}n^3 - 192m^2n^3 - \frac{1484}{5}n^5 + 300m^2n - 964mn^3 + 162mn^2 + 300n^2 + 760n^4m - 120n^5m + 32m^3n + 64m^2n^2 + \frac{1045}{2}n^4 - 144m^2.$$

Proof. We use the standard cut-method to compute our results. Let $\{S_1^i; 1 \leq i \leq m\}$, $\{S_2^i; 1 \leq i \leq m\}$, $\{S_1^k; 1 \leq k \leq 2m\}$, $\{S_2^k; 1 \leq k \leq 2m\}$, $\{S_1^j; 1 \leq j \leq m+n-1\}$, and $\{S_2^j; 1 \leq j \leq m+n-1\}$ be the four vertical and two diagonal cuts in $TiO_2(m, n)$ nanotubes respectively as shown in Fig. 2.

For every $1 \leq i \leq m$, we have $|S_1^i| = 2n$.

$$n_1(S_1^i) = 2n(6i - 5); n_2(S_1^i) = 12mn - 2n(6i - 5).$$

$$m_1(S_1^i) = (20n - 4)i - 18n + 3; m_2(S_1^i) = 20mn - 4m - 2n - (20n - 4)i + 18n - 3 - 2n.$$

Fig. 2. Cuts in $TiO_2(m, n)$ nanotube

For $1 \leq i \leq m$, we have $|S_2^i| = 2n$.

$$n_1(S_2^i) = 4n(3i - 1); n_2(S_2^i) = 12mn - 4n(3i - 1).$$

$$m_1(S_2^i) = (20n - 4)i - 8n + 1; m_2(S_2^i) = 20mn - 4m - 2n - (20n - 4)i + 8n - 1 - 2n.$$

For every $1 \leq k \leq 2m$, $|S_1^k| = 2n$.

$$n_1(S_1^k) = n(6k - 1); n_2(S_1^k) = 12mn - n(6k - 1).$$

$$m_1(S_1^k) = (10n - 3)k - 2n; m_2(S_1^k) = 20mn - 4m - 2n - (10n - 3)k + 2n - 2n.$$

For every $1 \leq k \leq 2m$, we have $|S_2^k| = 2n$.

$$n_1(S_2^k) = n_1(S_1^k); n_2(S_2^k) = n_2(S_1^k).$$

$$m_1(S_2^k) = m_1(S_1^k); m_2(S_2^k) = m_2(S_1^k).$$

For every $1 \leq j \leq n-1$, we have $|S_1^j| = 4j - 2$.

$$n_1(S_1^j) = 2(3j^2 - 2j); n_2(S_1^j) = 12mn - 2(3j^2 - 2j).$$

$$m_1(S_1^j) = 10j^2 - 11j + 2; m_2(S_1^j) = 20mn - 4m - 2n - 10j^2 + 11j - 2 - 4j + 2.$$

For every $n \leq j \leq m$, we have $|S_1^j| = 4n - 2$.

$$n_1(S_1^j) = 2(3(n-1)^2 - 2(n-1)) + (j-n+1)12n; n_2(S_1^j) = 12mn - 2(3(n-1)^2 - 2(n-1)) - (j-n+1)12n.$$

$$m_1(S_1^j) = 10n^2 - 11n + 2 + (j-n)(20n-4); m_2(S_1^j) = 20mn - 4m - 2n - 10n^2 + 11n - 2 - (j-n)(20n-4) - 4n + 2.$$

For every $m+1 \leq j \leq m+n-1$, we have $|S_1^j| = 4(m+n-j)$.

$$n_1(S_1^j) = 12mn - 6(m+n-j)^2 - 4(m+n-j); n_2(S_1^j) = 6(m+n-j)^2 + 4(m+n-j).$$

$$m_1(S_1^j) = 20mn - 4m - 2n - 10(m+n-j)^2 - 3(m+n-j); m_2(S_1^j) = 10(m+n-j)^2 + 3(m+n-j) + 4(m+n-j).$$

For every $1 \leq j \leq n-1$, we have $|S_2^j| = 4j - 2$.

$$n_1(S_2^j) = 2(3j^2 - j); n_2(S_2^j) = 12mn - 2(3j^2 - j).$$

$$m_1(S_2^j) = 10j^2 - 9j + 2; m_2(S_2^j) = 20mn - 4m - 2n - 10j^2 + 9j - 2 - 4j + 2.$$

For every $n \leq j \leq m$, we have $|S_2^j| = 4n - 2$.

$$n_1(S_2^j) = 2(3(n-1)^2 - (n-1)) + (j-n+1)12n; n_2(S_2^j) = 12mn - 2(3(n-1)^2 - (n-1)) - (j-n+1)12n.$$

$$m_1(S_2^j) = 10n^2 - 9n + 2 + (j-n)(20n-4); m_2(S_2^j) = 20mn - 4m - 2n - 10n^2 + 9n - 2 - (j-n)(20n-4) - 4n + 2.$$

For every $m+1 \leq j \leq m+n-1$, we have $|S_2^j| = 4(m+n-j)$

$$n_1(S_2^j) = 12mn - 6(m+n-j)^2 - 2(m+n-j); n_2(S_2^j) = 6(m+n-j)^2 + 2(m+n-j).$$

$$m_1(S_2^j) = 20mn - 4m - 2n - 10(m+n-j)^2 - 5(m+n-j); m_2(S_2^j) = 10(m+n-j)^2 + 5(m+n-j) + 4(m+n-j).$$

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Since, from [14] we have the following expression for the Wiener index $W(G)$:

$$W(G) = \sum_{i=1}^k n_1(F_i) \times n_2(F_i)$$

Therefore, by using the above data we have the following closed expression for Wiener index $W(G)$ for $TiO_2(m, n)$ nanotubes when $m > n$.

$$\begin{aligned} W(TiO_2(m, n)) &= \sum_{i=1}^m \{(2n(6i-5))(12mn-2n(6i-5))\} + \sum_{i=1}^m \{(4n(3i-1))(12mn-4n(3i-1))\} \\ &+ 2 \sum_{k=1}^{2m} \{(n(6k-1))(12mn-n(6k-1))\} + \sum_{j=1}^{n-1} \{(2(3j^2-2j))(12mn-2(3j^2-2j))\} \\ &+ \sum_{j=n}^m \{(2(2(3(n-1)^2-2(n-1))) + (j-n+1)12n)(12mn-2(2(3(n-1)^2-2(n-1))) \\ &- (j-n+1)12n)\} + \sum_{j=m+1}^{m+n-1} \{(12mn-6(m+n-j)^2-4(m+n-j))(6(m+n-j)^2 \\ &+ 4(m+n-j))\} + \sum_{j=1}^{n-1} \{(2(3j^2-j))(12mn-2(3j^2-j))\} + \sum_{j=n}^m \{(2(3(n-1)^2-(n-1)) \\ &+ (j-n+1)12n)(12mn-2(3(n-1)^2-(n-1)) - (j-n+1)12n)\} \\ &+ \sum_{j=m+1}^{m+n-1} \{(12mn-6(m+n-j)^2-2(m+n-j))(6(m+n-j)^2+2(m+n-j))\}. \end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\Rightarrow W(TiO_2(m, n)) = -164 + \frac{4112}{15}n + 192m^3n^2 + \frac{20}{3}n^3 - \frac{24}{5}n^5 + 24n^4m - 112n^2 - 20mn^2 + 112mn - 164m.$$

Since we have from [14]

$$Sz_v(G) = \sum_{i=1}^k |F_i| \{n_1(F_i) \times n_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for vertex-Szeged index $Sz_v(G)$ for $TiO_2(m, n)$ nanotubes $m > n$.

$$\begin{aligned} Sz_v(TiO_2(m, n)) &= \sum_{i=1}^m 2n \{(2n(6i-5))(12mn-2n(6i-5))\} + \sum_{i=1}^m 2n \{(4n(3i-1))(12mn-4n(3i-1))\} \\ &+ 2 \sum_{k=1}^{2m} 2n \{(n(6k-1))(12mn-n(6k-1))\} + \sum_{j=1}^{n-1} (4j-2) \{(2(3j^2-2j))(12mn-2(3j^2-2j))\} \\ &+ \sum_{j=n}^m (j-n+1) \{(2(2(3(n-1)^2-2(n-1))) + (j-n+1)12n)(12mn-2(2(3(n-1)^2-2(n-1))) \\ &- (j-n+1)12n)\} + \sum_{j=m+1}^{m+n-1} (m+n-j) \{(12mn-6(m+n-j)^2-4(m+n-j))(6(m+n-j)^2 \\ &+ 4(m+n-j))\} + \sum_{j=1}^{n-1} (2j-1) \{(2(3j^2-j))(12mn-2(3j^2-j))\} + \sum_{j=n}^m (j-n+1) \{(2(3(n-1)^2-(n-1)) \\ &+ (j-n+1)12n)(12mn-2(3(n-1)^2-(n-1)) - (j-n+1)12n)\} + \sum_{j=m+1}^{m+n-1} (m+n-j) \{(12mn-6(m+n-j)^2-2(m+n-j))(6(m+n-j)^2 \\ &+ 2(m+n-j))\}. \end{aligned}$$

$$\begin{aligned}
& -2j))\} + \sum_{j=n}^m (4n-2)\{2(3(n-1)^2 - 2(n-1)) + (j-n+1)12n\}(12mn - 2(3(n-1)^2 \\
& -2(n-1)) - (j-n+1)12n)\} + \sum_{j=m+1}^{m+n-1} 4(m+n-j)\{(12mn - 6(m+n-j)^2 \\
& -4(m+n-j))(6(m+n-j)^2 + 4(m+n-j))\} + \sum_{j=1}^{n-1} (4j-2)\{(2(3j^2 - j))(12mn \\
& -2(3j^2 - j))\} + \sum_{j=n}^m (4n-2)\{2(3(n-1)^2 - (n-1)) + (j-n+1)12n\}(12mn - 2(3(n-1)^2 \\
& - (n-1)) - (j-n+1)12n)\} + \sum_{j=m+1}^{m+n-1} 4(m+n-j)\{(12mn - 6(m+n-j)^2 \\
& -2(m+n-j))(6(m+n-j)^2 + 2(m+n-j))\}.
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned}
\Rightarrow Sz_v(TiO_2(m, n)) &= 328 - \frac{18092}{15}n + 480m^3n^3 - 96m^3n^2 - \frac{96}{5}n^5 + 48n^4m + 28n^4 + 464n^2m - \frac{1352}{3}n^3 \\
&\quad - 56mn^3 + 1320n^2 - 880mn + 328m.
\end{aligned}$$

Since, from [14] we have

$$Sz_e(G) = \sum_{i=1}^k |F_i| \{m_1(F_i) \times m_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge-Szeged index $Sz_e(G)$ for $TiO_2(m, n)$ nanotubes $m > n$.

$$\begin{aligned}
Sz_e(TiO_2(m, n)) &= \sum_{i=1}^m 2n\{((20n-4)i - 18n + 3)(20mn - 4m - 2n - (20n-4)i + 18n - 3 - 2n)\} \\
&\quad + \sum_{i=1}^m 2n\{((20n-4)i - 8n + 1)(20mn - 4m - 2n - (20n-4)i + 8n - 1 - 2n)\} \\
&\quad + 2 \sum_{k=1}^{2m} 2n\{((10n-3)k - 2n)(20mn - 4m - 2n - (10n-3)k + 2n - 2n)\} \\
&\quad + \sum_{j=1}^{n-1} (4j-2)\{(10j^2 - 11j + 2)(20mn - 4m - 2n - 10j^2 + 11j - 2 - 4j + 2)\} \\
&\quad + \sum_{j=n}^m (4n-2)\{(10n^2 - 11n + 2 + (j-n)(20n-4))(20mn - 4m - 2n - 10n^2 + 11n - 2 \\
&\quad - (j-n)(20n-4) - 4n + 2)\} + \sum_{j=m+1}^{m+n-1} 4(m+n-j)\{(20mn - 4m - 2n - 10(m+n-j)^2
\end{aligned}$$

$$\begin{aligned}
& -3(m+n-j)(10(m+n-j)^2 + 3(m+n-j) + 4(m+n-j))\} \\
& + \sum_{j=1}^{n-1} (4j-2)\{(10j^2 - 9j + 2)(20mn - 4m - 2n - 10j^2 + 9j - 2 - 4j + 2)\} \\
& + \sum_{j=n}^m (4n-2)\{(10n^2 - 9n + 2 + (j-n)(20n-4))(20mn - 4m - 2n - 10n^2 + 9n - 2 \\
& - (j-n)(20n-4) - 4n + 2)\} + \sum_{j=m+1}^{m+n-1} 4(m+n-j)\{(20mn - 4m - 2n - 10(m+n-j)^2 \\
& - 5(m+n-j)(10(m+n-j)^2 + 5(m+n-j) + 4(m+n-j))\}.
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned}
\Rightarrow Sz_e(TiO_2(m, n)) &= \frac{82}{3}n - \frac{2240}{3}m^3n^2 + 672m^2n^2 + \frac{416}{3}m^3n + \frac{4000}{3}m^3n^3 - 176n^5 - 960m^2n^3 - 184m^2n \\
&- \frac{32}{3}m^3 + 16m^2 + 236n^4 + \frac{2000}{3}n^4m + \frac{152}{3}n^3 - \frac{3056}{3}mn^3 + 412mn^2 - 138n^2 - \frac{64}{3}mn \\
&- \frac{16}{3}m.
\end{aligned}$$

Since, we have from [14]

$$Sz_{ev}(G) = \frac{1}{2} \sum_{i=1}^k |F_i| \{n_1(F_i) \times m_2(F_i) + n_2(F_i) \times m_1(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge vertex -Szeged index $Sz_{ev}(G)$ for $TiO_2(m, n)$ nanotubes $m > n$.

$$\begin{aligned}
Sz_{ev}(TiO_2(m, n)) &= \frac{1}{2} \left[\sum_{i=1}^m 2n\{(2n(6i-5))(20mn - 4m - 2n - (20n-4)i + 18n - 3 - 2n) + (12mn \right. \\
&- 2n(6i-5)((20n-4)i - 18n + 3))\} + \sum_{i=1}^m 2n\{(4n(3i-1))(20mn - 4m - 2n - (20n-4)i \\
&+ 8n - 1 - 2n) + (12mn - 4n(3i-1)((20n-4)i - 8n + 1))\} + 2 \sum_{k=1}^{2m} 2n\{(n(6k-1))(20mn \\
&- 4m - 2n - (10n-3)k) + 2n - 2n + (12mn - n(6k-1)((10n-3)k - 2n))\} \\
&+ \sum_{j=1}^{n-1} (4j-2)\{(2(3j^2 - 2j))(20mn - 4m - 2n - 10j^2 + 11j - 2 - 4j + 2) + (12mn \\
&- 2(3j^2 - 2j))(10j^2 - 11j + 2)\} + \sum_{j=n}^m (4n-2)\{(2(3(n-1)^2 - 2(n-1)) \\
&+ (j-n+1)12n)(20mn - 4m - 2n - 10n^2 + 11n - 2 - (j-n)(20n-4) + (12mn \\
&- 2(3(n-1)^2 - 2(n-1)) - (j-n+1)12n)(10n^2 - 11n + 2 + (j-n)(20n-4) - 4n + 2)\}
\end{aligned}$$

$$\begin{aligned}
& + \sum_{j=m+1}^{m+n-1} 4(m+n-j) \{ (12mn - 6(m+n-j)^2 - 4(m+n-j))(10(m+n-j)^2 \\
& + 3(m+n-j) + 4(m+n-j))(6(m+n-j)^2 + 4(m+n-j))(20mn - 4m - 2n \\
& - 10(m+n-j)^2 - 3(m+n-j)) \} + \sum_{j=1}^{n-1} (4j-2) \{ (2(3j^2-j))(20mn - 4m - 2n - 10j^2 \\
& + 9j - 2 - 4j + 2) + (12mn - 2(3j^2-j))(10j^2 - 9j + 2) \} + \sum_{j=n}^m (4n-2) \{ (2(3(n-1)^2 \\
& - (n-1)) + (j-n+1)12n)(20mn - 4m - 2n - 10n^2 + 9n - 2 - (j-n)(20n-4) - 4n \\
& + 2) \} + (12mn - 2(3(n-1)^2 - (n-1)) - (j-n+1)12n)(10n^2 - 9n + 2 \\
& + (j-n)(20n-4)) + \sum_{j=m+1}^{m+n-1} 4(m+n-j) \{ (12mn - 6(m+n-j)^2 \\
& - 2(m+n-j))(10(m+n-j)^2 + 5(m+n-j) + 4(m+n-j)) + (6(m+n-j))^2 \\
& + 2(m+n-j)(20mn - 4m - 2n - 10(m+n-j)^2 - 5(m+n-j)) \} \Big].
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned}
\Rightarrow Sz_{ev}(TiO_2(m, n)) &= 36 - \frac{4711}{30}n + 284mn + 960m^3n^3 - 352m^3n^2 - \frac{1334}{3}n^3 - 192m^2n^3 - \frac{1484}{5}n^5 \\
&+ 300m^2n - 964mn^3 + 162mn^2 + 300n^2 + 760n^4m - 120n^5m + 32m^3n + 64m^2n^2 \\
&+ \frac{1045}{2}n^4 - 144m^2.
\end{aligned}$$

□

The following corollary is an immediate consequence of the Theorem 2.0.1.

Corollary 2.1. *The total-Szeged index of $TiO_2(m, n)$ nanotubes for $m > n$ is as follows:*

$$\begin{aligned}
Sz_t(TiO_2(m, n)) &= 400 - \frac{22393}{15}n - 240n^5m + 416m^2n + \frac{608}{3}m^3n + 80n^6 - 1344m^2n^3 + 800m^2n^2 + 1200mn^2 \\
&+ \frac{6704}{3}n^4m - \frac{3944}{5}n^5 - \frac{9008}{3}mn^3 - \frac{1000}{3}mn + \frac{11200}{3}m^3n^3 - \frac{4640}{3}m^3n^2 + 1309n^4 - 272m^2 \\
&- \frac{32}{3}m^3 - \frac{3868}{3}n^3 + 1782n^2 + \frac{320}{3}m.
\end{aligned}$$

Proof. Since we have the following expression for the total-Szeged index

$$Sz_t(TiO_2(m, n)) = Sz_v(TiO_2(m, n)) + Sz_e(TiO_2(m, n)) + 2Sz_{ev}(TiO_2(m, n)).$$

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Therefore, from Theorem 2.0.1, we have

$$\begin{aligned}\Rightarrow Sz_t(TiO_2(m, n)) &= 328 - \frac{18092}{15}n + 480m^3n^3 - 96m^3n^2 + 28n^4 - \frac{96}{5}n^5 - \frac{1352}{3}n^3 + 464n^2m + 48n^4m \\ &\quad - 56mn^3 + 1320n^2 - 880mn + 328m + \frac{82}{3}n - \frac{2240}{3}m^3n^2 + 672m^2n^2 + \frac{416}{3}m^3n \\ &\quad + \frac{4000}{3}m^3n^3 - 176n^5 - 960m^2n^3 - 184m^2n - \frac{32}{3}m^3 + 16m^2 + 236n^4 + \frac{2000}{3}n^4m \\ &\quad + \frac{152}{3}n^3 + 760n^4m + 412mn^2 - \frac{3056}{3}mn^3 - 138n^2 - \frac{64}{3}mn - \frac{16}{3}m + 2(36 - \frac{4711}{30}n \\ &\quad + 284mn + 960m^3n^3 - 352m^3n^2 + 300m^2n - 964mn^3 + 162mn^2 + 300n^2 - \frac{1334}{3}n^3 \\ &\quad - 120n^5m + 32m^3n - 192m^2n^3 + 64m^2n^2 - 144m^2 + \frac{1045}{2}n^4 - \frac{1484}{5}n^5 + 40n^6 - 108m).\end{aligned}$$

After some calculations and simplification, we have

$$\begin{aligned}\Rightarrow Sz_t(TiO_2(m, n)) &= 400 - \frac{22393}{15}n - 240n^5m + 416m^2n + \frac{608}{3}m^3n + 80n^6 - 1344m^2n^3 + 800m^2n^2 \\ &\quad + 1200mn^2 + \frac{6704}{3}n^4m - \frac{3944}{5}n^5 - \frac{9008}{3}mn^3 - \frac{1000}{3}mn + \frac{11200}{3}m^3n^3 - \frac{4640}{3}m^3n^2 \\ &\quad + 1309n^4 - 272m^2 - \frac{32}{3}m^3 - \frac{3868}{3}n^3 + 1782n^2 + \frac{320}{3}m.\end{aligned}$$

□

In the next theorem, we compute the exact expression of the Wiener index and variants of Szeged index of $TiO_2(m, n)$ nanotubes for $m < n$.

Theorem 2.0.2. For every positive integer $m < n$, the exact expressions of the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:

$$\bullet W(TiO_2(m, n)) = -\frac{24}{5}m^5 - 20m^2n + 24m^4n + 144m^3n^2 + 48m^2n^3 + \frac{20}{3}m^3 - \frac{28}{15}m.$$

$$\bullet Sz_v(TiO_2(m, n)) = -\frac{32}{3}m^3 - 8m^2 - 56m^3n - 96m^4n + \frac{28}{15}m + 24m^2n + 28m^4 + 480m^3n^3 + \frac{144}{5}m^5.$$

$$\begin{aligned}\bullet Sz_e(TiO_2(m, n)) &= -\frac{2720}{3}m^3n^2 + 240m^2n^2 - \frac{952}{3}m^3n + \frac{4000}{3}m^3n^3 - \frac{208}{3}m^5 - \frac{1760}{3}m^2n^3 + 264m^2n \\ &\quad - \frac{188}{3}m^3 - 106m^2 + \frac{1040}{3}m^4n + 156m^4 - \frac{152}{3}mn^3 + \frac{200}{3}mn^2 - \frac{112}{3}mn + 22m.\end{aligned}$$

$$\bullet Sz_{ev}(TiO_2(m, n)) = -2mn - 120m^5n + \frac{76}{5}m^5 + 960m^3n^3 - 320m^3n^2 + 40m^6 - 16mn^3 - 18mn^2 - 92m^3n \\ - 80m^2n^3 + 28m^2n^2 + 82m^2n - \frac{170}{3}m^3 + \frac{93}{2}m^4 - 7m^2 + 64m^4n + \frac{269}{30}m.$$

Proof. Suppose that $\{S_1^i; 1 \leq i \leq m\}$, $\{S_2^i; 1 \leq i \leq m\}$, $\{S_1^k; 1 \leq k \leq 2m\}$, $\{S_2^k; 1 \leq k \leq 2m\}$, $\{S_1^j; 1 \leq j \leq m+n-1\}$, and $\{S_2^j; 1 \leq j \leq m+n-1\}$ be the four vertical and two diagonal cuts in $TiO_2(m, n)$ nanotubes respectively as shown in Fig. 2.

For every $1 \leq i \leq m$, we have $|S_1^i| = 2n$.

$$n_1(S_1^i) = 2n(6i - 5); n_2(S_1^i) = 12mn - 2n(6i - 5).$$

$$m_1(S_1^i) = (20n - 4)i - 18n + 3; m_2(S_1^i) = 20mn - 4m - 2n - (20n - 4)i + 18n - 3 - 2n.$$

For every $1 \leq i \leq m$, we have $|S_2^i| = 2n$.

$$n_1(S_2^i) = 4n(3i - 1); n_2(S_2^i) = 12mn - 4n(3i - 1)$$

$$m_1(S_2^i) = (20n - 4)i - 8n + 1; m_2(S_2^i) = 20mn - 4m - 2n - (20n - 4)i + 8n - 1 - 2n.$$

For every $1 \leq k \leq 2m$, we have $|S_1^k| = 2n$.

$$n_1(S_1^k) = n(6k - 1); n_2(S_1^k) = 12mn - n(6k - 1).$$

$$m_1(S_1^k) = (10n - 3)k - 2n; m_2(S_1^k) = 20mn - 4m - 2n - (10n - 3)k + 2n - 2n.$$

For every $1 \leq k \leq 2m$, we have $|S_2^k| = 2n$.

$$n_1(S_2^k) = n_1(S_1^k); n_2(S_2^k) = n_2(S_1^k).$$

$$m_1(S_2^k) = m_1(S_1^k); m_2(S_2^k) = m_2(S_1^k).$$

For every $1 \leq j \leq m$, we have $|S_1^j| = 4j - 2$.

$$n_1(S_1^j) = 2(3j^2 - 2j); n_2(S_1^j) = 12mn - 2(3j^2 - 2j).$$

$$m_1(S_1^j) = 10j^2 - 11j + 2; m_2(S_1^j) = 20mn - 4m - 2n - 10j^2 + 11j - 2 - 4j + 2.$$

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For every $m + 1 \leq j \leq n$; we have $|S_1^j| = 4m$.

$$n_1(S_1^j) = 2(3m^2 - 2m) + (j - m)12m; n_2(S_1^j) = 12mn - 2(3m^2 - 2m) - (j - m)12m.$$

$$m_1(S_1^j) = 10m^2 + 9m - 2 + (j - m - 1)(20m - 2); m_2(S_1^j) = 20mn - 4m - 2n - 10m^2 + 9m + 2 - (j - m - 1)(20m - 2) - 4m.$$

For every $n + 1 \leq j \leq m + n - 1$, we have $|S_1^j| = 4(m + n - j)$.

$$n_1(S_1^j) = 12mn - 6(m + n - j)^2 - 4(m + n - j); n_2(S_1^j) = 6(m + n - j)^2 + 4(m + n - j).$$

$$m_1(S_1^j) = 20mn - 4m - 2n - 10(m + n - j)^2 - 3(m + n - j); m_2(S_1^j) = 10(m + n - j)^2 + 3(m + n - j) + 4(m + n - j).$$

For every $1 \leq j \leq m$; we have $|S_2^j| = 4j - 2$.

$$n_1(S_2^j) = 2(3j^2 - j); n_2(S_2^j) = 12mn - 2(3j^2 - j).$$

$$m_1(S_2^j) = 10j^2 - 9j + 2; m_2(S_2^j) = 20mn - 4m - 2n - 10j^2 + 9j - 2 - 4j + 2.$$

For every $m + 1 \leq j \leq n$, we have $|S_2^j| = 4m$.

$$n_1(S_2^j) = 2(3m^2 - m) + (j - m)12m; n_2(S_2^j) = 12mn - 2(3m^2 - m) - (j - m)12m.$$

$$m_1(S_2^j) = 10m^2 + 11m - 2 + (j - m - 1)(20m - 2); m_2(S_2^j) = 20mn - 4m - 2n - 10m^2 + 11m + 2 - (j - m - 1)(20m - 2) - 4m.$$

For every $n + 1 \leq j \leq m + n - 1$, we have $|S_2^j| = 4(m + n - j)$.

$$n_1(S_2^j) = 12mn - 6(m + n - j)^2 - 2(m + n - j); n_2(S_2^j) = 6(m + n - j)^2 + 2(m + n - j).$$

$$m_1(S_2^j) = 20mn - 4m - 2n - 10(m + n - j)^2 - 5(m + n - j); m_2(S_2^j) = 10(m + n - j)^2 + 5(m + n - j) + 4(m + n - j).$$

Since, from we have the following expression for the Wiener index $W(G)$ from [14]

$$W(G) = \sum_{i=1}^k n_1(F_i) \times n_2(F_i)$$

Therefore, by using the above data we have the following closed expression for Wiener index $W(G)$ for $TiO_2(m, n)$ nanotubes for $m < n$.

$$\begin{aligned}
 W(TiO_2(m, n)) &= \sum_{i=1}^m \{(2n(6i-5))(12mn-2n(6i-5))\} + \sum_{i=1}^m \{(4n(3i-1))(12mn-4n(3i-1))\} \\
 &+ 2 \sum_{k=1}^{2m} \{(n(6k-1))(12mn-n(6k-1))\} + \sum_{j=1}^m \{(2(3j^2-2j))(12mn-2(3j^2-2j))\} \\
 &+ \sum_{j=m+1}^n \{(2(3m^2-2m)+(j-m)12m)(12mn-2(3m^2-2m)-(j-m)12m)\} \\
 &+ \sum_{j=n+1}^{m+n-1} \{(12mn-6(m+n-j)^2-4(m+n-j))(6(m+n-j)^2+4(m+n-j))\} \\
 &+ \sum_{j=1}^m \{(2(3j^2-j))(12mn-2(3j^2-j))\} + \sum_{j=m+1}^n \{(2(3m^2-m)+(j-m)12m)(12mn \\
 &-2(3m^2-m)-(j-m)12m)\} + \sum_{j=n+1}^{m+n-1} \{(12mn-6(m+n-j)^2 \\
 &-2(m+n-j))(6(m+n-j)^2+2(m+n-j))\}.
 \end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\Rightarrow W(TiO_2(m, n)) = -\frac{24}{5}m^5 - 20m^2n + 24m^4n + 144m^3n^2 + 48m^2n^3 + \frac{20}{3}m^3 - \frac{28}{15}m$$

Since, we have from [14]

$$Sz_v(G) = \sum_{i=1}^k |F_i| \{n_1(F_i) \times n_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for vertex-Szeged index $Sz_v(G)$ for $TiO_2(m, n)$ nanotubes when $m < n$.

$$\begin{aligned}
 Sz_v(TiO_2(m, n)) &= \sum_{i=1}^m 2n \{(2n(6i-5))(12mn-2n(6i-5))\} + \sum_{i=1}^m \{2n(4n(3i-1))(12mn-4n(3i-1))\} \\
 &+ 2 \sum_{k=1}^{2m} 2n \{(n(6k-1))(12mn-n(6k-1))\} + \sum_{j=1}^m (4j-2) \{(2(3j^2-2j))(12mn \\
 &-2(3j^2-2j))\} + \sum_{j=m+1}^n 4m \{(2(3m^2-2m)+(j-m)12m)(12mn-2(3m^2-2m)-(j \\
 &-m)12m)\} + \sum_{j=n+1}^{m+n-1} 4(m+n-j) \{(12mn-6(m+n-j)^2-4(m+n-j))(6(m+n-j)^2 \\
 &-2(m+n-j))\}.
 \end{aligned}$$

$$\begin{aligned}
& +4(m+n-j)\} + \sum_{j=1}^m (4j-2)\{(2(3j^2-j))(12mn-2(3j^2-j))\} + \sum_{j=m+1}^n \{4m(2(3m^2-m) \\
& +(j-m)12m)(12mn-2(3m^2-m)-(j-m)12m)\} + \sum_{j=n+1}^{m+n-1} 4(m+n-j)\{(12mn \\
& -6(m+n-j)^2-2(m+n-j))(6(m+n-j)^2+2(m+n-j))\}.
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\Rightarrow Sz_v(TiO_2(m, n)) = -\frac{32}{3}m^3 - 8m^2 - 56m^3n - 96m^4n + \frac{28}{15}m + 24m^2n + 28m^4 + 480m^3n^3 + \frac{144}{5}m^5.$$

Since, from [14] we have

$$Sz_e(G) = \sum_{i=1}^k |F_i| \{m_1(F_i) \times m_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge-Szeged index $Sz_e(G)$ for $TiO_2(m, n)$ nanotubes when $m < n$.

$$\begin{aligned}
Sz_e(TiO_2(m, n)) &= \sum_{i=1}^m 2n\{((20n-4)i-18n+3)(20mn-4m-2n-(20n-4)i+18n-3-2n)\} \\
&+ \sum_{i=1}^m 2n\{((20n-4)i-8n+1)(20mn-4m-2n-(20n-4)i+8n-1-2n)\} \\
&+ 2 \sum_{k=1}^{2m} 2n\{((10n-3)k-2n)(20mn-4m-2n-(10n-3)k+2n-2n)\} \\
&+ \sum_{j=1}^m (4j-2)\{(10j^2-11j+2)(20mn-4m-2n-10j^2+11j-2-4j+2)\} \\
&+ \sum_{j=m+1}^n 4m\{(10m^2+9m-2+(j-m-1)(20m-2))(20mn-4m-2n-10m^2-9m+2 \\
&- (j-m-1)(20m-2)-4m)\} + \sum_{j=n+1}^{m+n-1} 4(m+n-j)\{(20mn-4m-2n-10(m+n-j))^2 \\
&- 3(m+n-j)(10(m+n-j)^2+3(m+n-j)+4(m+n-j))\} + \sum_{j=1}^m (4j-2)\{(10j^2 \\
&- 9j+2)(20mn-4m-2n-10j^2+9j-4j)\} + \sum_{j=m+1}^n 4m\{(10m^2+11m-2+(j-m \\
&- 1)(20m-2))(20mn-4m-2n-10m^2-11m+2-(j-m-1)(20m-2)-4m)\} \\
&+ \sum_{j=n+1}^{m+n-1} 4(m+n-j)\{(20mn-4m-2n-10(m+n-j))^2-5(m+n-j)(10(m+n-j)^2 \\
&+ 5(m+n-j)+4(m+n-j))\}.
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\Rightarrow Sz_e(TiO_2(m, n)) = -\frac{2720}{3}m^3n^2 + 240m^2n^2 - \frac{952}{3}m^3n + \frac{4000}{3}m^3n^3 - \frac{208}{3}m^5 - \frac{1760}{3}m^2n^3 + 264m^2n - \frac{188}{3}m^3 - 106m^2 + \frac{1040}{3}m^4n + 156m^4 - \frac{152}{3}mn^3 + \frac{200}{3}mn^2 - \frac{112}{3}mn + 22m.$$

Since we have

$$Sz_{ev}(G) = \frac{1}{2} \sum_{i=1}^k |F_i| \{n_1(F_i) \times m_2(F_i) + n_2(F_i) \times m_1(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge vertex -Szeged index $Sz_{ev}(G)$ for $TiO_2(m, n)$ nanotubes when $m < n$.

$$\begin{aligned} Sz_{ev}(TiO_2(m, n)) &= \frac{1}{2} \left[\sum_{i=1}^m 2n \{ (2n(6i-5))(20mn-4m-2n-(20n-4)i+18n-3-2n) + (12mn \right. \\ &\quad - 2n(6i-5))((20n-4)i-18n+3) \} + \sum_{i=1}^m 2n \{ (4n(3i-1))(20mn-4m-2n-(20n-4)i \\ &\quad + 8n-1-2n) + (12mn-4n(3i-1))((20n-4)i-8n+1) \} + 2 \sum_{k=1}^{2m} 2n \{ (n(6k-1))(20mn \\ &\quad - 4m-2n-(10n-3)k+2n-2n) + (12mn-n(6k-1))((10n-3)k-2n) \} \\ &\quad + \sum_{j=1}^m (4j-2) \{ (2(3j^2-2j))(20mn-4m-2n-10j^2+11j-2-4j+2) + (12mn \\ &\quad - 2(3j^2-2j))(10j^2-11j+2) \} + \sum_{j=m+1}^n 4m \{ (2(3m^2-2m) + (j-m)12m)(20mn-4m \\ &\quad - 2n-10m^2-9m+2-(j-m-1)(20m-2)-4m) + (12mn-2(3m^2-2m)-(j \\ &\quad -m)12m)(10m^2+9m-2+(j-m-1)(20m-2)) \} + \sum_{j=n+1}^{m+n-1} 4(m+n-j) \{ (12mn \\ &\quad - 6(m+n-j)^2-4(m+n-j))(10(m+n-j)^2+3(m+n-j)+4(m+n-j)) \\ &\quad + (6(m+n-j)^2+4(m+n-j))(20mn-4m-2n-10(m+n-j)^2-3(m+n-j)) \} \\ &\quad + \sum_{j=1}^m (4j-2) \{ (2(3j^2-j))(20mn-4m-2n-10j^2+9j-2-4j+2) + (12mn \\ &\quad - 2(3j^2-j))(10j^2-9j+2) \} + \sum_{j=m+1}^n 4m \{ (2(3m^2-m) + (j-m)12m)(20mn-4m-2n \\ &\quad - 10m^2-11m+2-(j-m-1)(20m-2)-4m) + (12mn-2(3m^2-m)-(j \\ &\quad -m)12m)(10m^2+11m-2+(j-m-1)(20m-2)) \} \\ &\quad + \sum_{j=n+1}^{m+n-1} 4(m+n-j) \{ (12mn-6(m+n-j)^2-2(m+n-j))(10(m+n-j)^2 \\ &\quad + 5(m+n-j)+4(m+n-j) + (6(m+n-j)^2+2(m+n-j))(20mn-4m-2n \end{aligned}$$

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$$-10(m+n-j)^2 - 5(m+n-j))\} \Bigg].$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned} \Rightarrow Sz_{ev}(TiO_2(m, n)) &= -2mn - 120m^5n + \frac{76}{5}m^5 + 960m^3n^3 - 320m^3n^2 + 40m^6 - 16mn^3 - 18mn^2 - 92m^3n \\ &\quad - 80m^2n^3 + 28m^2n^2 + 82m^2n - \frac{170}{3}m^3 + \frac{93}{2}m^4 - 7m^2 + 64m^4n + \frac{269}{30}m. \end{aligned}$$

□

The following corollary is an immediate consequence of the Theorem 2.0.2.

Corollary 2.2. *The total-Szeged index of $TiO_2(m, n)$ for $m < n$ is as follows :*

$$\begin{aligned} Sz_t(TiO_2(m, n)) &= 452m^2n - \frac{1672}{3}m^3n - \frac{2240}{3}m^2n^3 + 296m^2n^2 + \frac{92}{3}mn^2 - \frac{248}{3}mn^3 - \frac{124}{3}mn + \frac{11200}{3}m^3n^3 \\ &\quad - \frac{4640}{3}m^3n^2 + 277m^4 + 80m^6 - \frac{152}{15}m^5 - 128m^2 - \frac{560}{3}m^3 - 240m^5n + \frac{209}{5}m + \frac{1136}{3}m^4n. \end{aligned}$$

Proof. Since we have the following expression for the total-Szeged index.

$$Sz_t(TiO_2(m, n)) = Sz_v(TiO_2(m, n)) + Sz_e(TiO_2(m, n)) + 2Sz_{ev}(TiO_2(m, n))$$

Therefore, from Theorem 2.0.1, we have

$$\begin{aligned} \Rightarrow Sz_t(TiO_2(m, n)) &= -\frac{32}{3}m^3 - 8m^2 - 56m^3n - 96m^4n + \frac{28}{15}m + 24m^2n + 480m^3n^3 + 28m^4 + \frac{144}{5}m^5 \\ &\quad - \frac{2720}{3}m^3n^2 + 240m^2n^2 - \frac{952}{3}m^3n + \frac{4000}{3}m^3n^3 - \frac{1760}{3}m^2n^3 + 264m^2n - \frac{188}{3}m^3 \\ &\quad - 106m^2 + \frac{1040}{3}m^4n - \frac{152}{3}mn^3 + \frac{200}{3}mn^2 - \frac{112}{3}mn + 22m + 156m^4 - \frac{208}{3}m^5 \\ &\quad + 2(-2mn + \frac{76}{5}m^5 - 120m^5n + 960m^3n^3 - 320m^3n^2 + 82m^2n + 40m^6 - 16mn^3 - 18mn^2 \\ &\quad - 92m^3n - 80m^2n^3 + 28m^2n^2 - \frac{170}{3}m^3 + \frac{93}{2}m^4 - 7m^2 + 64m^4n + \frac{269}{30}m). \end{aligned}$$

After some calculations and simplifications, we have

$$\begin{aligned} \Rightarrow Sz_t(TiO_2(m, n)) &= 452m^2n - \frac{1672}{3}m^3n - \frac{2240}{3}m^2n^3 + 296m^2n^2 + \frac{92}{3}mn^2 - \frac{248}{3}mn^3 - \frac{124}{3}mn \\ &\quad + \frac{11200}{3}m^3n^3 - \frac{4640}{3}m^3n^2 + 277m^4 + 80m^6 - \frac{152}{15}m^5 - 128m^2 - \frac{560}{3}m^3 - 240m^5n \end{aligned}$$

$$+\frac{209}{5}m + \frac{1136}{3}m^4n.$$

□

In the next theorem, we compute the exact expressions of the Wiener index and variants of Szeged index of $TiO_2(m, n)$ nanotubes for $m = n$.

Theorem 2.0.3. *For every positive integer $m = n$, the exact expressions of the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:*

$$\begin{aligned} \bullet W(TiO_2(m, n)) &= -\frac{14}{15}n + 36mn^3 + 144m^3n^2 + 48m^4n - 36m^3n - 12m^2n - 8m^2 + \frac{16}{3}n^3 - \frac{72}{5}n^5 + 48n^4m \\ &\quad + \frac{28}{3}m^3 + 14m^4 + 8n^2 - 12mn^2 - 18n^4 - \frac{72}{5}m^5 - \frac{14}{15}m \end{aligned}$$

$$\begin{aligned} \bullet Sz_v(TiO_2(m, n)) &= -\frac{116}{15}n - 12n^2 + \frac{136}{3}n^3 - 56m^3 + 4m^2 - 192m^4n + \frac{432}{5}m^5 - 72mn^3 - \frac{288}{5}n^5 + 40n^4 \\ &\quad - 48n^6 - 48m^6 + 144n^5m + 96n^4m + 4m^4 + 144m^5n + \frac{48}{5}m + 48m^2n + 288m^3n^3 - 24n^2m \end{aligned}$$

$$\begin{aligned} \bullet Sz_e(TiO_2(m, n)) &= 22n + 800m^3n^3 - \frac{800}{3}n^6 - \frac{800}{3}m^3n^2 + 800n^5m - \frac{1600}{3}n^4m + 64n^5 + \frac{908}{3}n^4 + \frac{32}{3}m^3n \\ &\quad - 84n^3 - 24m^2n - 480m^2n^3 + 176m^2n^2 - \frac{1384}{3}mn^3 + 376mn^2 - 90n^2 - \frac{160}{3}mn \end{aligned}$$

$$\begin{aligned} \bullet Sz_{ev}(TiO_2(m, n)) &= -\frac{259}{30}n + 240m^5n + \frac{552}{5}m^5 + 640m^3n^3 - 128m^3n^2 - 80m^6 + 104m^2n - 92mn^3 - 46mn^2 \\ &\quad - 7n^2 + \frac{160}{3}n^3 + 96n^4m + 120n^5m - 56m^3n - 48m^2n^3 + 16m^2n^2 - 108m^3 + 62m^4 - 2m^2 \\ &\quad + \frac{49}{2}n^4 - \frac{336}{5}n^5 - 40n^6 - 284m^4n + \frac{88}{5}m \end{aligned}$$

Proof. For every $1 \leq i \leq m$, we have $|S_1^i| = 2n$.

$$n_1(S_1^i) = 2n(6i - 5); n_2(S_1^i) = 12mn - 2n(6i - 5).$$

$$m_1(S_1^i) = (20n - 4)i - 18n + 3; m_2(S_1^i) = 20mn - 4m - 2n - (20n - 4)i + 18n - 3 - 2n.$$

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For every $1 \leq i \leq m$, we have $|S_2^i| = 2n$.

$$n_1(S_2^i) = 4n(3i - 1); n_2(S_2^i) = 12mn - 4n(3i - 1).$$

$$m_1(S_2^i) = (20n - 4)i - 8n + 1; m_2(S_2^i) = 20mn - 4m - 2n - (20n - 4)i + 8n + 1 - 2n.$$

For every $1 \leq k \leq 2m$, we have $|S_1^k| = 2n$.

$$n_1(S_1^k) = n(6k - 1); n_2(S_1^k) = 12mn - n(6k - 1).$$

$$m_1(S_1^k) = (10n - 3)k - 2n; m_2(S_1^k) = 20mn - 4m - 2n - (10n - 3)k$$

For every $1 \leq k \leq 2m$, we have $|S_2^k| = 2n$.

$$n_1(S_2^k) = n_1(S_1^k); n_2(S_2^k) = n_2(S_1^k).$$

$$m_1(S_2^k) = m_1(S_1^k); m_2(S_2^k) = m_2(S_1^k).$$

For every $1 \leq j \leq n$, we have $|S_1^j| = 4j - 2$.

$$n_1(S_1^j) = 2(3j^2 - 2j); n_2(S_1^j) = 12mn - 2(3j^2 - 2j)$$

$$m_1(S_1^j) = 10j^2 - 11j + 2; m_2(S_1^j) = 20mn - 4m - 2n - 10j^2 + 11j - 2 - 4j + 2.$$

For every $n + 1 \leq j \leq m + n - 1$, we have $|S_1^j| = 4(m + n - j)$.

$$n_1(S_1^j) = 12mn - 6(m + n - j)^2 - 4(m + n - j); n_2(S_1^j) = 6(m + n - j)^2 + 4(m + n - j).$$

$$m_1(S_1^j) = 20mn - 4m - 2n - 10(m + n - j)^2 - 3(m + n - j); m_2(S_1^j) = 10(m + n - j)^2 + 3(m + n - j) + 4(m + n - j).$$

For every $1 \leq j \leq n$, we have $|S_2^j| = 4j - 2$.

$$n_1(S_2^j) = 2(3j^2 - j); n_2(S_2^j) = 12mn - 2(3j^2 - j).$$

$$m_1(S_2^j) = 10j^2 - 9j + 2; m_2(S_2^j) = 20mn - 4m - 2n - 10j^2 + 9j - 2 - 4j + 2.$$

For every $n + 1 \leq j \leq m + n - 1$, we have $|S_2^j| = 4(m + n - j)$.

$$n_1(S_2^j) = 12mn - 6(m + n - j)^2 - 2(m + n - j); n_2(S_2^j) = 6(m + n - j)^2 + 2(m + n - j).$$

$$m_1(S_2^j) = 20mn - 4m - 2n - 10(m + n - j)^2 - 5(m + n - j); m_2(S_2^j) = 10(m + n - j)^2 + 5(m + n - j) + 4(m + n - j).$$

Since, we have from [14]

$$W(G) = \sum_{i=1}^k n_1(F_i) \times n_2(F_i)$$

Therefore, by using the above data we have the following closed expression for Wiener index $W(G)$ for $TiO_2(m, n)$ nanotubes for $m = n$.

$$\begin{aligned} W(TiO_2(m, n)) &= \sum_{i=1}^m \{(2n(6i - 5))(12mn - 2n(6i - 5))\} + \sum_{i=1}^m \{(4n(3i - 1))(12mn - 4n(3i - 1))\} \\ &+ 2 \sum_{k=1}^{2m} \{(n(6k - 1))(12mn - n(6k - 1))\} + \sum_{j=1}^n \{(2(3j^2 - 2j))(12mn - 2(3j^2 - 2j))\} \\ &+ \sum_{j=n+1}^{m+n-1} \{(12mn - 6(m + n - j)^2 - 4(m + n - j))(6(m + n - j)^2 + 4(m + n - j))\} \\ &+ \sum_{j=1}^n \{(2(3j^2 - j))(12mn - 2(3j^2 - j))\} + \sum_{j=n+1}^{m+n-1} \{(12mn - 6(m + n - j)^2 \\ &- 2(m + n - j))(6(m + n - j)^2 + 2(m + n - j))\}. \end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned} \Rightarrow W(TiO_2(m, n)) &= -\frac{14}{15}n + 36mn^3 + 144m^3n^2 + 48m^4n - 36m^3n - 12m^2n - 8m^2 + \frac{16}{3}n^3 - \frac{72}{5}n^5 + 48n^4m \\ &+ \frac{28}{3}m^3 + 14m^4 + 8n^2 - 12mn^2 - 18n^4 - \frac{72}{5}m^5 - \frac{14}{15}m. \end{aligned}$$

Since we have from [14]

$$Sz_v(G) = \sum_{i=1}^k |F_i| \{n_1(F_i) \times n_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for vertex-Szeged index $Sz_v(G)$ for $TiO_2(m, n)$ nanotubes when $m = n$.

$$Sz_v(TiO_2(m, n)) = \sum_{i=1}^m 2n \{(2n(6i - 5))(12mn - 2n(6i - 5))\} + \sum_{i=1}^m \{2n(4n(3i - 1))(12mn - 4n(3i - 1))\}$$

$$\begin{aligned}
& +2 \sum_{k=1}^{2m} 2n\{(n(6k-1))(12mn-n(6k-1))\} + \sum_{j=1}^n \{(4j-2)(2(3j^2-2j))(12mn-2(3j^2-2j))\} \\
& + \sum_{j=n+1}^{m+n-1} 4(m+n-j)\{(12mn-6(m+n-j)^2-4(m+n-j))(6(m+n-j)^2 \\
& +4(m+n-j))\} + \sum_{j=1}^n (4j-2)\{(2(3j^2-j))(12mn-2(3j^2-j))\} \\
& + \sum_{j=n+1}^{m+n-1} 4(m+n-j)\{(12mn-6(m+n-j)^2-2(m+n-j))(6(m+n-j)^2 \\
& +2(m+n-j))\}
\end{aligned}$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned}
\Rightarrow Sz_v(TiO_2(m, n)) &= -\frac{116}{15}n - 12n^2 + \frac{136}{3}n^3 - 56m^3 + 4m^2 - 192m^4n + \frac{432}{5}m^5 - 72mn^3 - \frac{288}{5}n^5 + 40n^4 \\
&- 48n^6 - 48m^6 + 144n^5m + 96n^4m + 4m^4 + 144m^5n + \frac{48}{5}m + 48m^2n + 288m^3n^3 \\
&- 24n^2m
\end{aligned}$$

Since, from [14] we have

$$Sz_e(G) = \sum_{i=1}^k |F_i| \{m_1(F_i) \times m_2(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge-Szeged index $Sz_e(G)$ for $TiO_2(m, n)$ nanotubes when $m = n$.

$$\begin{aligned}
Sz_e(TiO_2(m, n)) &= \sum_{i=1}^m 2n\{((20n-4)i-18n+3)(20mn-4m-2n-(20n-4)i+18n-3-2n)\} \\
&+ \sum_{i=1}^m 2n\{((20n-4)i-8n+1)(20mn-4m-2n-(20n-4)i+8n-1-2n)\} \\
&+ 2 \sum_{k=1}^{2m} 2n\{((10n-3)k-2n)(20mn-4m-2n-(10n-3)k)+2n-2n\} \\
&+ \sum_{j=1}^n (4j-2)\{(10j^2-11j+2)(20mn-4m-2n-10j^2+11j-2-4j+2)\} \\
&+ \sum_{j=n+1}^{m+n-1} \{4(m+n-j)(20mn-4m-2n-10(m+n-j)^2-3(m+n-j))(10(m+n-j)^2 \\
&+3(m+n-j)+4(m+n-j))\} + \sum_{j=1}^n \{(4j-2)(10j^2-9j+2)(20mn-4m-2n-10j^2
\end{aligned}$$

$$+9j-2-4j+2)\} + \sum_{j=n+1}^{m+n-1} \{4(m+n-j)(20mn-4m-2n-10(m+n-j))^2 \\ -5(m+n-j)(10(m+n-j))^2 + 5(m+n-j) + 4(m+n-j)\}.$$

After some calculations and simplification, we have the following closed form

$$\Rightarrow Sz_e(TiO_2(m, n)) = 22n + 800m^3n^3 - \frac{800}{3}n^6 - \frac{800}{3}m^3n^2 + 800n^5m + 64n^5 - \frac{1600}{3}n^4m + \frac{908}{3}n^4 \\ + \frac{32}{3}m^3n - 84n^3 - 24m^2n - 480m^2n^3 + 176m^2n^2 - \frac{1384}{3}mn^3 + 376mn^2 - 90n^2 \\ - \frac{160}{3}mn$$

Since we have

$$Sz_{ev}(G) = \frac{1}{2} \sum_{i=1}^k |F_i| \{n_1(F_i) \times m_2(F_i) + n_2(F_i) \times m_1(F_i)\}$$

Therefore, by using the above data we have the following closed expression for edge vertex -Szeged index $Sz_{ev}(G)$ for $TiO_2(m, n)$ nanotubes when $m = n$.

$$Sz_{ev}(TiO_2(m, n)) = \frac{1}{2} \left[\sum_{i=1}^m 2n \{ (2n(6i-5))(20mn-4m-2n-(20n-4)i+18n-3-2n) + (12mn \right. \\ \left. -2n(6i-5))((20n-4)i-18n+3) \} + \sum_{i=1}^m 2n \{ (4n(3i-1))(20mn-4m-2n-(20n-4)i \right. \\ \left. +8n-1-2n) + (12mn-4n(3i-1))((20n-4)i-8n+1) \} + 2 \sum_{k=1}^{2m} 2n \{ (n(6k-1))(20mn \right. \\ \left. -4m-2n-(10n-3)k+2n-2n) + (12mn-n(6k-1))((10n-3)k-2n) \} \right. \\ \left. + \sum_{j=1}^n (4j-2) \{ (2(3j^2-2j))(20mn-4m-2n-10j^2+11j-2-4j+2) + (12mn \right. \\ \left. -2(3j^2-2j))(10j^2-11j+2) \} + \sum_{j=n+1}^{m+n-1} 4(m+n-j) \{ (12mn-6(m+n-j))^2 \right. \\ \left. -4(m+n-j)(10(m+n-j))^2 + 3(m+n-j) + 4(m+n-j) \} + (6(m+n-j))^2 \right. \\ \left. + 4(m+n-j)(20mn-4m-2n-10(m+n-j))^2 - 3(m+n-j) \} \right. \\ \left. + \sum_{j=1}^n (4j-2) \{ (2(3j^2-j))(20mn-4m-2n-10j^2+9j-2-4j+2) + (12mn \right. \\ \left. -2(3j^2-j))(10j^2-9j+2) \} + \sum_{j=n+1}^{m+n-1} 4(m+n-j) \{ (12mn-6(m+n-j))^2 \right. \\ \left. -2(m+n-j)(10(m+n-j))^2 + 5(m+n-j) + 4(m+n-j) \} + (6(m+n-j))^2 \right]$$

$$+2(m+n-j)(20mn-4m-2n-10(m+n-j)^2-5(m+n-j))\}\Bigg].$$

After some calculations and simplification, we have the following closed form

$$\begin{aligned}\Rightarrow Sz_{ev}(TiO_2(m,n)) &= -\frac{259}{30}n + 240m^5n + \frac{552}{5}m^5 + 640m^3n^3 - 128m^3n^2 - 80m^6 + 104m^2n - 92mn^3 \\ &\quad - 46mn^2 - 7n^2 + \frac{160}{3}n^3 + 96n^4m + 120n^5m - 56m^3n - 48m^2n^3 + 16m^2n^2 - 108m^3 \\ &\quad + 62m^4 - 2m^2 + \frac{49}{2}n^4 - \frac{336}{5}n^5 - 40n^6 - 284m^4n + \frac{88}{5}m.\end{aligned}$$

□

The following corollary is an immediate consequence of the Theorem 2.0.2.

Corollary 2.3. *The total-Szeged index of $TiO_2(m,n)$ nanotubes for $m = n$ is as follows :*

$$\begin{aligned}Sz_t(TiO_2(m,n)) &= -3n + 1184n^5m + 232m^2n - \frac{304}{3}m^3n - 576m^2n^3 + 208m^2n^2 + 260mn^2 - \frac{736}{3}n^4m \\ &\quad - \frac{2152}{3}mn^3 - \frac{160}{3}mn + 2368m^3n^3 - \frac{1568}{3}m^3n^2 + 128m^4 - 208m^6 + \frac{1536}{5}m^5 - \frac{1184}{3}n^6 \\ &\quad - 128n^5 + \frac{1175}{3}n^4 - 272m^3 + 68n^3 - 116n^2 + 624m^5n - 760m^4n + \frac{224}{5}m.\end{aligned}$$

Proof. Since we have the following expression for the total-Szeged index.

$$Sz_t(TiO_2(m,n)) = Sz_v(TiO_2(m,n)) + Sz_e(TiO_2(m,n)) + 2Sz_{ev}(TiO_2(m,n))$$

Therefore, by Theorem 2.0.3 we have

$$\begin{aligned}\Rightarrow Sz_t(TiO_2(m,n)) &= -\frac{116}{15}n - 12n^2 + \frac{136}{3}n^3 - 56m^3 + 4m^2 - 192m^4n + \frac{432}{5}m^5 - 72mn^3 - \frac{288}{5}n^5 + 40n^4 \\ &\quad - 48n^6 - 48m^6 + 144n^5m + 96n^4m + 4m^4 + 144m^5n + \frac{48}{5}m + 48m^2n + 288m^3n^3 \\ &\quad - 24n^2m + 22n + 800m^3n^3 - \frac{800}{3}n^6 - \frac{800}{3}m^3n^2 + 800n^5m - \frac{1600}{3}n^4m + 64n^5 + \frac{908}{3}n^4 \\ &\quad + \frac{32}{3}m^3n - 84n^3 - 24m^2n - 480m^2n^3 + 176m^2n^2 - \frac{1384}{3}mn^3 + 376mn^2 - 90n^2 \\ &\quad - \frac{160}{3}mn + 2\left(-\frac{259}{30}n + 240m^5n + \frac{552}{5}m^5 + 640m^3n^3 - 128m^3n^2 - 80m^6 + 104m^2n \right. \\ &\quad \left. - 92mn^3 - 46mn^2 - 7n^2 + \frac{160}{3}n^3 + 96n^4m + 120n^5m - 56m^3n - 48m^2n^3 + 16m^2n^2 \right. \\ &\quad \left. - 108m^3 + 62m^4 - 2m^2 + \frac{49}{2}n^4 - \frac{336}{5}n^5 - 40n^6 - 284m^4n + \frac{88}{5}m\right).\end{aligned}$$

After some calculations and simplifications, we get

$$\begin{aligned} \Rightarrow Sz_t(TiO_2(m, n)) &= -3n + 1184n^5m + 232m^2n - \frac{304}{3}m^3n - 576m^2n^3 + 208m^2n^2 + 260mn^2 - \frac{736}{3}n^4m \\ &\quad - \frac{2152}{3}mn^3 - \frac{160}{3}mn + 2368m^3n^3 - \frac{1568}{3}m^3n^2 + 128m^4 - 208m^6 + \frac{1536}{5}m^5 - \frac{1184}{3}n^6 \\ &\quad - 128n^5 + \frac{1175}{3}n^4 - 272m^3 + 68n^3 - 116n^2 + 624m^5n - 760m^4n + \frac{224}{5}m. \end{aligned}$$

□

3 Conclusion

In this paper, we have studied the Wiener index, vertex-Szeged index, edge-Szeged index and total-Szeged Index of single walled titania nanotubes $TiO_2(m, n)$ by using the cut-method for every positive integer m and n and derived the analytical closed expressions for Wiener index and variants of Szeged index for $TiO_2(m, n)$ nanotubes for the first time.

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Appendix –Maple Codes

For every positive integer $m > n$, the Maple codes for the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:

$$\begin{aligned} \bullet W(TiO_2(m, n)) &= identify(expand(sum(2 * n * (6 * i - 5) * (12 * m * n - 2 * n * (6 * i - 5)), i = 1..m) \\ &+ sum(4 * n * (3 * i - 1) * (12 * m * n - 4 * n * (3 * i - 1)), i = 1..m) \\ &+ 2 * (sum(n * (6 * k - 1) * (12 * m * n - n * (6 * k - 1)), k = 1..2 * m)) \\ &+ sum((2 * (3 * j^2 - 2 * j)) * (12 * m * n - 2 * (3 * j^2 - 2 * j)), j = 1..n - 1) \\ &+ sum((2 * (3 * (n - 1)^2 - 2 * (n - 1)) + ((j - n + 1) * 12) * n) * (12 * m * n \\ &- 2 * (3 * (n - 1)^2 - 2 * (n - 1)) - ((j - n + 1) * 12) * n), j = n..m) \\ &+ sum((12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n - j)) * (6 * (m + n - j)^2 \\ &+ 4 * (m + n - j)), j = m + 1..m + n - 1) + sum((2 * (3 * j^2 - j)) * (12 * m * n \\ &- 2 * (3 * j^2 - j)), j = 1..n - 1) + sum((2 * (3 * (n - 1)^2 - n + 1) \\ &+ ((j - n + 1) * 12) * n) * (12 * m * n - 2 * (3 * (n - 1)^2 - n + 1) \\ &- ((j - n + 1) * 12) * n), j = n..m) + sum((12 * m * n - 6 * (m + n - j)^2 \\ &- 2 * (m + n - j)) * (6 * (m + n - j)^2 + 2 * (m + n - j)), j = m + 1..m + n - 1))). \end{aligned}$$

$$\begin{aligned} \bullet Sz_v(TiO_2(m, n)) &= identify(expand(sum((2 * n * (2 * n * (6 * i - 5))) * (12 * m * n \\ &- 2 * n * (6 * i - 5)), i = 1..m) + sum((2 * n * (4 * n * (3 * i - 1))) * (12 * m * n \\ &- 4 * n * (3 * i - 1)), i = 1..m) + 2 * (sum((2 * n * (n * (6 * k - 1))) * (12 * m * n \\ &- n * (6 * k - 1)), k = 1..2 * m)) + sum((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (12 * m * n \\ &- 2 * (3 * j^2 - 2 * j)), j = 1..n - 1) + sum((4 * n - 2) * (2 * (3 * (n - 1)^2 - 2 * (n - 1)) \\ &+ ((j - n + 1) * 12) * n) * (12 * m * n - 2 * (3 * (n - 1)^2 - 2 * (n - 1)) \\ &- ((j - n + 1) * 12) * n), j = n..m) + sum((4 * (m + n - j)) * (12 * m * n - 6 * (m + n - j)^2 \\ &- 4 * (m + n - j)) * (6 * (m + n - j)^2 + 4 * (m + n - j)), j = m + 1..m + n - 1) \\ &+ sum((4 * j - 2) * (2 * (3 * j^2 - j)) * (12 * m * n - 2 * (3 * j^2 - j)), j = 1..n - 1) \\ &+ sum((4 * n - 2) * (2 * (3 * (n - 1)^2 - n + 1) + ((j - n + 1) * 12) * n) * (12 * m * n \end{aligned}$$

$$\begin{aligned}
& -2 * (3 * (n - 1)^2 - n + 1) - ((j - n + 1) * 12) * n, j = n..m) \\
& + \text{sum}((4 * (m + n - j)) * (12 * m * n - 6 * (m + n - j)^2 \\
& - 2 * (m + n - j)) * (6 * (m + n - j)^2 + 2 * (m + n - j)), j = m + 1..m + n - 1))).
\end{aligned}$$

$$\begin{aligned}
\bullet Sz_e(TiO_2(m, n)) &= \text{denti}fy(\text{expand}(\text{sum}(2 * n * ((20 * n - 4) * i - 8 * n + 1) * (20 * m * n - 4 * m - 2 * n \\
& - (20 * n - 4) * i + 8 * n - 1 - 2 * n), i = 1..m) + \text{sum}(2 * n * ((20 * n - 4) * i - 18 * n \\
& + 3) * (20 * m * n - 4 * m - 2 * n - (20 * n - 4) * i + 18 * n - 3 - 2 * n), i = 1..m) \\
& + 2 * (\text{sum}(2 * n * ((10 * n - 3) * k - 2 * n) * (20 * m * n - 4 * m - 2 * n \\
& - (10 * n - 3) * k), k = 1..2 * m)) + \text{sum}((4 * j - 2) * (10 * j^2 - 11 * j + 2) * (-10 * j^2 \\
& + 20 * m * n + 11 * j - 4 * m - 2 * n - 4 * j), j = 1..n - 1) + \text{sum}((4 * n - 2) * (10 * n^2 \\
& - 11 * n + 2 + (j - n) * (20 * n - 4)) * (20 * m * n - 10 * n^2 - 4 * m - 2 * n + 11 * n \\
& - (j - n) * (20 * n - 4) - 4 * n), j = n..m) + \text{sum}((4 * (m + n - j)) * (20 * m * n - 4 * m \\
& - 2 * n - 10 * (m + n - j)^2 - 3 * (m + n - j)) * (10 * (m + n - j)^2 + 7 * (m + n \\
& - j)), j = m + 1..m + n - 1) + \text{sum}((4 * j - 2) * (10 * j^2 - 9 * j + 2) * (-10 * j^2 \\
& + 20 * m * n + 9 * j - 4 * m - 2 * n - 4 * j), j = 1..n - 1) + \text{sum}((4 * n - 2) * (10 * n^2 \\
& - 9 * n + 2 + (j - n) * (20 * n - 4)) * (20 * m * n - 10 * n^2 - 4 * m - 2 * n + 9 * n \\
& - (j - n) * (20 * n - 4) - 4 * n), j = n..m) + \text{sum}((4 * (m + n - j)) * (20 * m * n - 4 * m \\
& - 2 * n - 10 * (m + n - j)^2 - 5 * (m + n - j)) * (10 * (m + n - j)^2 \\
& + 9 * (m + n - j)), j = m + 1..m + n - 1))).
\end{aligned}$$

$$\begin{aligned}
\bullet Sz_{ev}(TiO_2(m, n)) &= \text{identi}fy(\text{expand}(1/2 * (\text{sum}(2 * n * (2 * n * (6 * i - 5) * (20 * m * n - 4 * m - 2 * n \\
& - (20 * n - 4) * i + 18 * n + 3 - 2 * n) + (12 * m * n - 2 * n * (6 * i - 5)) * ((20 * n - 4) * i \\
& - 18 * n + 3)), i = 1..m) + \text{sum}(2 * n * (4 * n * (3 * i - 1) * (20 * m * n - 4 * m - 2 * n \\
& - (20 * n - 4) * i + 8 * n - 1 - 2 * n) + (12 * m * n - 4 * n * (3 * i - 1)) * ((20 * n - 4) * i \\
& - 8 * n + 1)), i = 1..m) + 2 * (\text{sum}(2 * n * (n * (6 * k - 1) * (20 * m * n - 4 * m - 2 * n \\
& - (10 * n - 3) * k + 2 * n - 2 * n) + (12 * m * n - n * (3 * k - 1)) * ((10 * n - 3) * k \\
& - 2 * n)), k = 1..2 * m)) + \text{sum}((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (-10 * j^2 + 20 * m * n
\end{aligned}$$

$$\begin{aligned}
& +11*j - 4*m - 2*n - 4*j) + (12*m*n - 2*(3*j^2 - 2*j)) * (10*j^2 - 11*j \\
& +2), j = 1..n-1) + sum((4*n - 2) * ((2*(3*(n-1)^2 - 2*(n-1)) + ((j-n \\
& +1)*12)*n) * (20*m*n - 10*n^2 - 4*m - 2*n + 11*n - 2 - (j-n) * (20*n - 4) \\
& -4*n + 2) + (12*m*n - 2*(3*(n-1)^2 - 2*(n-1)) - ((j-n \\
& +1)*12)*n) * (10*n^2 - 11*n + 2 + (j-n) * (20*n - 4))), j = n..m) \\
& +sum((4*(m+n-j)) * ((12*m*n - 6*(m+n-j)^2 - 4*(m+n-j)) * (10*(m \\
& +n-j)^2 + 7*(m+n-j)) + (6*(m+n-j)^2 + 4*(m+n-j)) * (20*m*n - 4*m \\
& -2*n - 10*(m+n-j)^2 - 3*(m+n-j))), j = m+1..m+n-1) + sum((4*j \\
& -2) * (2*(3*j^2 - j)) * (-10*j^2 + 20*m*n + 9*j - 4*m - 2*n - 4*j) \\
& + (12*m*n - 2*(3*j^2 - j)) * (10*j^2 - 9*j + 2), j = 1..n-1) + sum((4*n \\
& -2) * ((2*(3*(n-1)^2 - n + 1) + ((j-n+1)*12)*n) * (20*m*n - 10*n^2 - 4*m \\
& -2*n + 9*m - 2 - (j-n) * (20*n - 4) - 4*n + 2) + (12*m*n - 2*(3*(n-1)^2 \\
& -n + 1) - ((j-n+1)*12)*n) * (10*n^2 - 9*m + 2 + (j-n) * (20*n \\
& -4))), j = n..m) + sum((4*(m+n-j)) * ((12*m*n - 6*(m+n-j)^2 \\
& -2*(m+n-j)) * (10*(m+n-j)^2 + 9*(m+n-j)) + (6*(m+n-j)^2 \\
& +2*(m+n-j)) * (20*m*n - 4*m - 2*n - 10*(m+n-j)^2 \\
& -5*(m+n-j))), j = m+1..m+n-1))).
\end{aligned}$$

The maple code for the total-Szeged index of $TiO_2(m, n)$ nanotubes for $m > n$ is as follows:

$$\begin{aligned}
Sz_t(TiO_2(m, n)) &= identify(expand(328 - (18092/15)*n + 480*m^3*n^3 - 96*m^3*n^2 + 28*n^4 \\
&- (96/5)*n^5 + 464*m*n^2 + 48*n^4*m - 56*m*n^3 - (1352/3)*n^3 + 1320*n^2 \\
&- 880*m*n + 328*m + (82/3)*n - (2240/3)*m^3*n^2 + 672*m^2*n^2 + (416/3)*m^3*n \\
&+ (4000/3)*m^3*n^3 - 960*m^2*n^3 - 184*m^2*n - (32/3)*m^3 + 16*m^2 + 236*n^4 \\
&- 176*n^5 + (2000/3)*n^4*m + (152/3)*n^3 - (3056/3)*m*n^3 + 412*m*n^2 - 138*n^2 \\
&- (64/3)*m*n - (16/3)*m + 2*(36 - (4711/30)*n + 284*m*n + 960*m^3*n^3 \\
&- 352*m^3*n^2 + 300*m^2*n - 964*m*n^3 + 162*m*n^2 + 300*n^2 - (1334/3)*n^3 \\
&+ 760*n^4*m - 120*n^5*m + 32*m^3*n - 192*m^2*n^3 + 64*m^2*n^2 - 144*m^2
\end{aligned}$$

$$+(1045/2) * n^4 - (1484/5) * n^5 + 40 * n^6 - 108 * m)).$$

For every positive integer $m < n$, the Maple codes for the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:

$$\begin{aligned} \bullet W(TiO_2(m, n)) &= identify(expand(sum(2 * n * (6 * i - 5) * (12 * m * n - 2 * n * (6 * i - 5)), i = 1..m) \\ &+ sum(4 * n * (3 * i - 1) * (12 * m * n - 4 * n * (3 * i - 1)), i = 1..m) \\ &+ 2 * (sum(n * (6 * k - 1) * (12 * m * n - n * (6 * k - 1)), k = 1..2 * m)) + sum((2 * (3 * j^2 \\ &- 2 * j)) * (12 * m * n - 2 * (3 * j^2 - 2 * j)), j = 1..m) + sum((2 * (3 * m^2 - 2 * m) + ((j \\ &- m) * 12) * m) * (12 * m * n - 2 * (3 * m^2 - 2 * m) - ((j - m) * 12) * m), j = m + 1..n) \\ &+ sum((12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n - j)) * (6 * (m + n - j)^2 + 4 * (m \\ &+ n - j)), j = n + 1..m + n - 1) + sum((2 * (3 * j^2 - j)) * (12 * m * n - 2 * (3 * j^2 \\ &- j)), j = 1..m) + sum((2 * (3 * m^2 - m) + ((j - m) * 12) * m) * (12 * m * n - 2 * (3 * m^2 \\ &- m) - ((j - m) * 12) * m), j = m + 1..n) + sum((12 * m * n - 6 * (m + n - j)^2 - 2 * (m \\ &+ n - j)) * (6 * (m + n - j)^2 + 2 * (m + n - j)), j = n + 1..m + n - 1))). \end{aligned}$$

$$\begin{aligned} \bullet Sz_v(TiO_2(m, n)) &= identify(expand(sum((2 * n * (2 * n * (6 * i - 5))) * (12 * m * n - 2 * n * (6 * i \\ &- 5)), i = 1..m) + sum((2 * n * (4 * n * (3 * i - 1))) * (12 * m * n - 4 * n * (3 * i \\ &- 1)), i = 1..m) + 2 * (sum((2 * n * (n * (6 * k - 1))) * (12 * m * n - n * (6 * k \\ &- 1)), k = 1..2 * m)) + sum((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (12 * m * n - 2 * (3 * j^2 \\ &- 2 * j)), j = 1..m) + sum(4 * m * (2 * (3 * m^2 - 2 * m) + ((j - m) * 12) * m) * (12 * m * n \\ &- 2 * (3 * m^2 - 2 * m) - ((j - m) * 12) * m), j = m + 1..n) + sum((4 * (m + n \\ &- j)) * (12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n - j)) * (6 * (m + n - j)^2 \\ &+ 4 * (m + n - j)), j = n + 1..m + n - 1) + sum((4 * j - 2) * (2 * (3 * j^2 - j)) * (12 * m * n \\ &- 2 * (3 * j^2 - j)), j = 1..m) + sum(4 * m * (2 * (3 * m^2 - m) \\ &+ ((j - m) * 12) * m) * (12 * m * n - 2 * (3 * m^2 - m) - ((j - m) * 12) * m), j = m + 1..n) \\ &+ sum((4 * (m + n - j)) * (12 * m * n - 6 * (m + n - j)^2 - 2 * (m \\ &+ n - j)) * (6 * (m + n - j)^2 + 2 * (m + n - j)), j = n + 1..m + n - 1))). \end{aligned}$$

$$\begin{aligned}
\bullet Sz_e(TiO_2(m, n)) &= identify(expand(sum(2 * n * ((20 * n - 4) * i - 8 * n + 1) * (20 * m * n - 4 * m - 2 * n \\
&\quad - (20 * n - 4) * i + 8 * n - 1 - 2 * n), i = 1..m) + sum(2 * n * ((20 * n - 4) * i - 18 * n \\
&\quad + 3) * (20 * m * n - 4 * m - 2 * n - (20 * n - 4) * i + 18 * n - 3 - 2 * n), i = 1..m) \\
&\quad + 2 * (sum(2 * n * ((10 * n - 3) * k - 2 * n) * (20 * m * n - 4 * m - 2 * n - (10 * n \\
&\quad - 3) * k), k = 1..2 * m)) + sum((4 * j - 2) * (10 * j^2 - 11 * j + 2) * (-10 * j^2 + 20 * m * n \\
&\quad + 11 * j - 4 * m - 2 * n - 4 * j), j = 1..m) + sum(4 * m * (10 * m^2 + 9 * m - 2 + (j - m \\
&\quad - 1) * (20 * m - 2)) * (-10 * m^2 + 20 * m * n - 4 * m - 2 * n - 9 * m + 2 - (j - m \\
&\quad - 1) * (20 * m - 2) - 4 * m), j = m + 1..n) + sum((4 * (m + n - j)) * (20 * m * n - 4 * m \\
&\quad - 2 * n - 10 * (m + n - j)^2 - 3 * (m + n - j)) * (10 * (m + n - j)^2 + 7 * (m + n \\
&\quad - j)), j = n + 1..m + n - 1) + sum((4 * j - 2) * (10 * j^2 - 9 * j + 2) * (-10 * j^2 \\
&\quad + 20 * m * n + 9 * j - 4 * m - 2 * n - 4 * j), j = 1..m) + sum(4 * m * (10 * m^2 + 11 * m - 2 \\
&\quad + (j - m - 1) * (20 * m - 2)) * (-10 * m^2 + 20 * m * n - 4 * m - 2 * n - 11 * m + 2 \\
&\quad - (j - m - 1) * (20 * m - 2) - 4 * m), j = m + 1..n) + sum((4 * (m + n - j)) * (20 * m * n \\
&\quad - 4 * m - 2 * n - 10 * (m + n - j)^2 - 5 * (m + n - j)) * (10 * (m + n - j)^2 \\
&\quad + 9 * (m + n - j)), j = n + 1..m + n - 1))). \\
\bullet Sz_{ev}(TiO_2(m, n)) &= identify(expand(1/2 * (sum(2 * n * (2 * n * (6 * i - 5) * (20 * m * n - 4 * m - 2 * n \\
&\quad - (20 * n - 4) * i + 18 * n + 3 - 2 * n) + (12 * m * n - 2 * n * (6 * i - 5)) * ((20 * n - 4) * i \\
&\quad - 18 * n + 3)), i = 1..m) + sum(2 * n * (4 * n * (3 * i - 1) * (20 * m * n - 4 * m - 2 * n \\
&\quad - (20 * n - 4) * i + 8 * n + 1 - 2 * n) + (12 * m * n - 4 * n * (3 * i - 1)) * ((20 * n - 4) * i \\
&\quad - 8 * n + 1)), i = 1..m) + 2 * (sum(2 * n * (n * (6 * k - 1) * (20 * m * n - 4 * m \\
&\quad - 2 * n - (10 * n - 3) * k + 2 * n - 2 * n) + (12 * m * n - n * (3 * k - 1)) * ((10 * n - 3) * k \\
&\quad - 2 * n)), k = 1..2 * m)) + sum((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (-10 * j^2 + 20 * m * n \\
&\quad + 11 * j - 4 * m - 2 * n - 4 * j) + (12 * m * n - 2 * (3 * j^2 - 2 * j)) * (10 * j^2 - 11 * j \\
&\quad + 2), j = 1..m) + sum(4 * m * ((2 * (3 * m^2 - 2 * m) + ((j - m) * 12) * m) * (-10 * m^2 \\
&\quad + 20 * m * n - 4 * m - 2 * n - 9 * m + 2 - (j - m - 1) * (20 * m - 2) - 4 * m) + (12 * m * n \\
&\quad - 2 * (3 * m^2 - 2 * m) - ((j - m) * 12) * m) * (10 * m^2 + 9 * m - 2 + (j - m - 1) * (20 * m
\end{aligned}$$

$$\begin{aligned}
& -2))), j = m + 1..n) + \text{sum}((4 * (m + n - j)) * ((12 * m * n - 6 * (m + n - j)^2 - 4 * (m \\
& + n - j)) * (10 * (m + n - j)^2 + 7 * (m + n - j)) + (6 * (m + n - j)^2 + 4 * (m + n \\
& - j)) * (20 * m * n - 4 * m - 2 * n - 10 * (m + n - j)^2 - 3 * (m + n \\
& - j))), j = n + 1..m + n - 1) + \text{sum}((4 * j - 2) * (2 * (3 * j^2 - j)) * (-10 * j^2 + 20 * m * n \\
& + 9 * j - 4 * m - 2 * n - 4 * j) + (12 * m * n - 2 * (3 * j^2 - j)) * (10 * j^2 - 9 * j \\
& + 2), j = 1..m) + \text{sum}(4 * m * ((2 * (3 * m^2 - m) + ((j - m) * 12) * m) * (-10 * m^2 \\
& + 20 * m * n - 4 * m - 2 * n - 11 * m + 2 - (j - m - 1) * (20 * m - 2) - 4 * m) \\
& + (12 * m * n - 2 * (3 * m^2 - m) - ((j - m) * 12) * m) * (10 * m^2 + 11 * m - 2 + (j \\
& - m - 1) * (20 * m - 2))), j = m + 1..n) + \text{sum}((4 * (m + n - j)) * ((12 * m * n \\
& - 6 * (m + n - j)^2 - 2 * (m + n - j)) * (10 * (m + n - j)^2 + 9 * (m + n - j)) \\
& + (6 * (m + n - j)^2 + 2 * (m + n - j)) * (20 * m * n - 4 * m - 2 * n - 10 * (m + n - j)^2 \\
& - 5 * (m + n - j))), j = n + 1..m + n - 1))).
\end{aligned}$$

The maple code for the total-Szeged index of $TiO_2(m, n)$ nanotubes for $m < n$ is as follows:

$$\begin{aligned}
Sz_t(TiO_2(m, n)) &= \text{identify}(\text{expand}(-(116/15) * n - 48 * m^6 - 48 * n^6 + 288 * m^3 * n^3 + 48 * m^2 * n \\
&- 24 * n^2 * m + 144 * m^5 * n + 144 * n^5 * m - 192 * m^4 * n + 96 * n^4 * m + (432/5) * m^5 \\
&- (288/5) * n^5 + 4 * m^4 + 40 * n^4 - 56 * m^3 + 4 * m^2 + (136/3) * n^3 - 72 * m * n^3 - 12 * n^2 \\
&+ (48/5) * m + 22 * n - (800/3) * m^3 * n^2 + 176 * m^2 * n^2 + (32/3) * m^3 * n + 800 * m^3 * n^3 \\
&- 480 * m^2 * n^3 - 24 * m^2 * n + (908/3) * n^4 + 64 * n^5 - (1600/3) * n^4 * m + 800 * n^5 * m \\
&- 84 * n^3 - (1384/3) * m * n^3 + 376 * n^2 * m - 90 * n^2 - (160/3) * m * n - (800/3) * n^6 \\
&+ 2 * (- (259/30) * n + 240 * m^5 * n + (552/5) * m^5 + 640 * m^3 * n^3 - 128 * m^3 * n^2 \\
&+ 104 * m^2 * n - 80 * m^6 - 92 * m * n^3 - 46 * n^2 * m - 7 * n^2 + (160/3) * n^3 + 96 * n^4 * m \\
&+ 120 * n^5 * m - 56 * m^3 * n - 48 * m^2 * n^3 + 16 * m^2 * n^2 - 108 * m^3 + 62 * m^4 - 2 * m^2 \\
&+ (49/2) * n^4 - (336/5) * n^5 - 40 * n^6 - 284 * m^4 * n + (88/5) * m))).
\end{aligned}$$

For every positive integer $m = n$, the Maple codes for the Wiener index and variants of Szeged index in $TiO_2(m, n)$ nanotubes are as follows:

$$\begin{aligned} \bullet W(TiO_2(m, n)) &= identify(expand(sum(2 * n * (6 * i - 5) * (12 * m * n - 2 * n * (6 * i - 5)), i = 1..m) \\ &+ sum(4 * n * (3 * i - 1) * (12 * m * n - 4 * n * (3 * i - 1)), i = 1..m) + 2 * (sum(n * (6 * k \\ &- 1) * (12 * m * n - n * (6 * k - 1)), k = 1..2 * m)) + sum((2 * (3 * j^2 - 2 * j)) * (12 * m * n \\ &- 2 * (3 * j^2 - 2 * j)), j = 1..n) + sum((12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n \\ &- j)) * (6 * (m + n - j)^2 + 4 * (m + n - j)), j = n + 1..m + n - 1) + sum((2 * (3 * j^2 \\ &- j)) * (12 * m * n - 2 * (3 * j^2 - j)), j = 1..n) + sum((12 * m * n - 6 * (m + n - j)^2 \\ &- 2 * (2 * m + n - j)) * (6 * (m + n - j)^2 + 2 * (m + n - j)), j = n + 1..m + n - 1))). \end{aligned}$$

$$\begin{aligned} \bullet Sz_v(TiO_2(m, n)) &= identify(expand(sum((2 * n * (2 * n * (6 * i - 5))) * (12 * m * n - 2 * n * (6 * i \\ &- 5)), i = 1..m) + sum((2 * n * (4 * n * (3 * i - 1))) * (12 * m * n - 4 * n * (3 * i \\ &- 1)), i = 1..m) + 2 * (sum((2 * n * (n * (6 * k - 1))) * (12 * m * n - n * (6 * k \\ &- 1)), k = 1..2 * m)) + sum((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (12 * m * n - 2 * (3 * j^2 \\ &- 2 * j)), j = 1..n) + sum((4 * (m + n - j)) * (12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n \\ &- j)) * (6 * (m + n - j)^2 + 4 * (m + n - j)), j = n + 1..m + n - 1) + sum((4 * j \\ &- 2) * (2 * (3 * j^2 - j)) * (12 * m * n - 2 * (3 * j^2 - j)), j = 1..n) + sum((4 * (m + n \\ &- j)) * (12 * m * n - 6 * (m + n - j)^2 - 2 * (m + n - j)) * (6 * (m + n - j)^2 \\ &+ 2 * (m + n - j)), j = n + 1..m + n - 1))). \end{aligned}$$

$$\begin{aligned} \bullet Sz_e(TiO_2(m, n)) &= identify(expand(sum(2 * n * ((20 * n - 4) * i - 8 * n + 1) * (20 * m * n - 4 * m - 2 * n \\ &- (20 * n - 4) * i + 8 * n - 1 - 2 * n), i = 1..m) + sum(2 * n * ((20 * n - 4) * i - 18 * n \\ &+ 3) * (20 * m * n - 4 * m - 2 * n - (20 * n - 4) * i + 18 * n - 3 - 2 * n), i = 1..m) \\ &+ 2 * (sum(2 * n * ((10 * n - 3) * k - 2 * n) * (20 * m * n - 4 * m - 2 * n - (10 * n \\ &- 3) * k), k = 1..2 * m)) + sum((4 * j - 2) * (10 * j^2 - 11 * j + 2) * (-10 * j^2 + 20 * m * n \\ &+ 11 * j - 4 * m - 2 * n - 4 * j), j = 1..n) + sum((4 * (m + n - j)) * (20 * m * n - 4 * m \end{aligned}$$

$$\begin{aligned}
& -2 * n - 10 * (m + n - j)^2 - 3 * (m + n - j)) * (10 * (m + n - j)^2 + 7 * (m + n \\
& - j)), j = m + 1..m + n - 1) + \text{sum}((4 * j - 2) * (10 * j^2 - 9 * j + 2) * (-10 * j^2 \\
& + 20 * m * n + 9 * j - 4 * m - 2 * n - 4 * j), j = 1..n) \\
& + \text{sum}((4 * (m + n - j)) * (20 * m * n - 4 * m - 2 * n - 10 * (m + n - j)^2 - 5 * (m \\
& + n - j)) * (10 * (m + n - j)^2 + 9 * (m + n - j)), j = m + 1..m + n - 1))).
\end{aligned}$$

$$\begin{aligned}
\bullet Sz_{ev}(TiO_2(m, n)) &= \text{identify}(\text{expand}(1/2 * (\text{sum}(2 * n * (2 * n * (6 * i - 5) * (20 * m * n - 4 * m - 2 * n \\
& - (20 * n - 4) * i + 18 * n + 3 - 2 * n) + (12 * m * n - 2 * n * (6 * i - 5)) * ((20 * n - 4) * i \\
& - 18 * n + 3)), i = 1..m) + \text{sum}(2 * n * (4 * n * (3 * i - 1) * (20 * m * n - 4 * m - 2 * n \\
& - (20 * n - 4) * i + 8 * n - 1 - 2 * n) + (12 * m * n - 4 * n * (3 * i - 1)) * ((20 * n - 4) * i \\
& - 8 * n + 1)), i = 1..m) + 2 * (\text{sum}(2 * n * (n * (6 * k - 1) * (20 * m * n - 4 * m - 2 * n \\
& - (10 * n - 3) * k + 2 * n - 2 * n) + (12 * m * n - n * (3 * k - 1)) * ((10 * n - 3) * k \\
& - 2 * n)), k = 1..2 * m)) + \text{sum}((4 * j - 2) * (2 * (3 * j^2 - 2 * j)) * (-10 * j^2 + 20 * m * n \\
& + 11 * j - 4 * m - 2 * n - 4 * j) + (12 * m * n - 2 * (3 * j^2 - 2 * j)) * (10 * j^2 - 11 * j \\
& + 2), j = 1..n) + \text{sum}((4 * (m + n - j)) * ((12 * m * n - 6 * (m + n - j)^2 - 4 * (m + n \\
& - j)) * (10 * (m + n - j)^2 + 7 * (m + n - j)) + (6 * (m + n - j)^2 + 4 * (m + n \\
& - j)) * (20 * m * n - 4 * m - 2 * n - 10 * (m + n - j)^2 - 3 * (m + n \\
& - j))), j = n + 1..m + n - 1) + \text{sum}((4 * j - 2) * (2 * (3 * j^2 - j)) * (-10 * j^2 \\
& + 20 * m * n + 9 * j - 4 * m - 2 * n - 2 - 4 * j + 2) + (12 * m * n - 2 * (3 * j^2 \\
& - j)) * (10 * j^2 - 9 * j + 2), j = 1..n) + \text{sum}((4 * (m + n - j)) * ((12 * m * n \\
& - 6 * (m + n - j)^2 - 2 * (m + n - j)) * (10 * (m + n - j)^2 + 9 * (m + n - j)) \\
& + (6 * (m + n - j)^2 + 2 * (m + n - j)) * (20 * m * n - 4 * m - 2 * n - 10 * (m + n - j)^2 \\
& - 5 * (m + n - j))), j = n + 1..m + n - 1))).
\end{aligned}$$

The maple code for the total-Szeged index of $TiO_2(m, n)$ nanotubes for $m = n$ is as follows:

$$\begin{aligned}
Sz_t(TiO_2(m, n)) &= \text{identify}(\text{expand}(-(32/3) * m^3 - 8 * m^2 - 56 * m^3 * n - 96 * m^4 * n + (28/15) * m \\
& + 24 * m^2 * n + 480. * m^3 * n^3 + 28 * m^4 + (144/5) * m^5 - (2720/3) * m^3 * n^2 + 240 * m^2 * n^2
\end{aligned}$$

$$\begin{aligned}
& -(952/3) * m^3 * n + (4000/3) * m^3 * n^3 - (1760/3) * m^2 * n^3 + 264 * m^2 * n - (188/3) * m^3 \\
& -106 * m^2 + (1040/3) * m^4 * n - (152/3) * m * n^3 + (200/3) * m * n^2 - (112/3) * m * n \\
& +22 * m + 156 * m^4 - (208/3) * m^5 + 2 * (-2 * m * n - 120 * m^5 * n + (76/5) * m^5 \\
& +960 * m^3 * n^3 - 320 * m^3 * n^2 + 82 * m^2 * n + 40 * m^6 - 16 * m * n^3 - 18 * m * n^2 \\
& -92 * m^3 * n - 80 * m^2 * n^3 + 28 * m^2 * n^2 - (170/3) * m^3 + (93/2) * m^4 - 7 * m^2 \\
& +64 * m^4 * n + (269/30) * m))).
\end{aligned}$$

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