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THE VERTEX SZEGED INDEX OF TITANIA CARBON NANOTUBES TiO_2 *(m,n)*

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ABSTRACT: Let *G=(V,E)* be a simple connected molecular graph in chemical graph theory, where the vertex set and edge set of G denoted by *V(G)* and *E(G)* respectively and its vertices correspond to the atoms and the edges correspond to the bonds. A topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. In this paper, the vertex Szeged index of *Titania* carbon Nanotubes $TiO_2(m,n)$ is computed.

INTRODUCTION: Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph [1-8].

We first describe some notations which will be kept throughout. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by *V(G)* and *E(G)*, respectively.

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Suppose G is a connected molecular graph and $x, y \in V(G)$. The distance $d(x,y)$ between x and y is defined as the length of a minimum path between x and y. Many topological indices there are in mathematical chemistry and several applications of them have been found in physical, chemical and pharmaceutical models and other properties of molecules. A topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The oldest nontrivial topological index is the Wiener index which was introduced by Chemist *Harold Wiener* [9]. The *Wiener index* is defined as

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

where $d(u,v)$ be the distance between two vertices *u* and *v*.

In 1994, Ivan Gutman defined a new topological index and named it Szeged index (Sz) index and the Szeged index of the graph G is defined as [10, 11].

$$Sz(G)=\sum_{e\in E(G)}\left(n_u(e|G)\times n_v(e|G)\right)$$

where $n_u(e|G)$ is the number of vertices of G lying closer to u than v and $n_v(e|G)$ is the number of vertices of G lying closer to v than u. Notice that vertices equidistance from u and v are not taken into account.

The aim of this paper is to compute the vertex Szeged index of Titania carbon Nanotubes $TiO_2(m,n)$. Throughout this paper, our notation is standard. For further study of some applications of Szeged indices in nanotechnology can be finding in the paper series [12-18].

RESULTS AND DISCUSSION:

In this present section, the vertex Szeged index of Titania carbon Nanotubes $TiO_2(m,n)$. The graph of the Titania Nanotubes $TiO_2(m,n)$ 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 Nanotubes. We encourage the reader to consult papers [19-30], for further study and more information of Titania Nanotubes TiO_2.

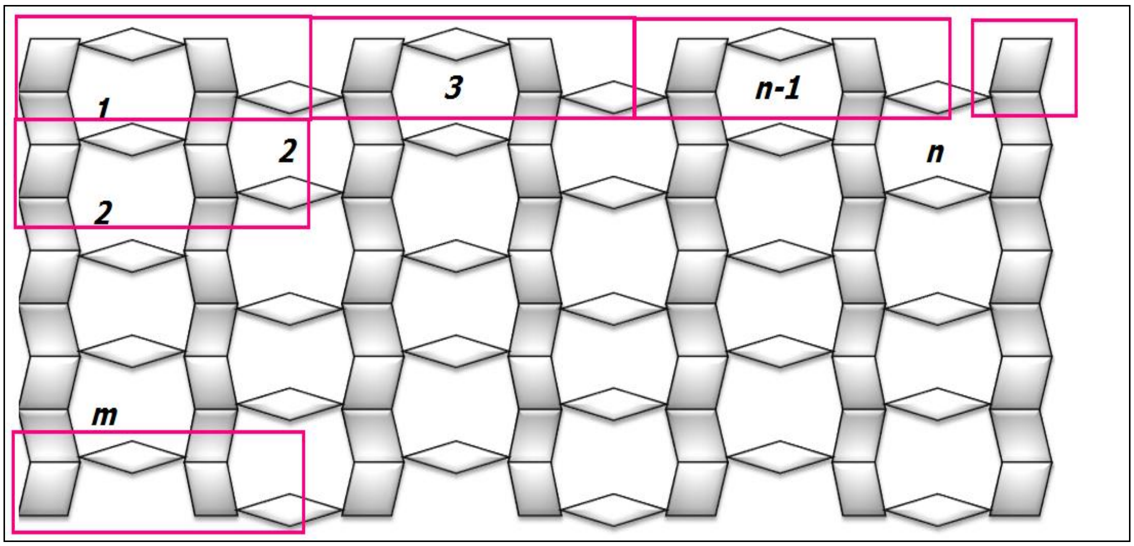

FIG. 1: THE TITANIA PLANAR NANOTUBES $TiO_2(m,n)$ $\forall m,n\in\mathbb{N}$.

Theorem 1: Let $TiO_2(m,n)$ be the Titania Nanotubes for a non-negative integers *m,n*. Then vertex Szeged index of $TiO_2(m,n)$ is equal to:

$$SZ_v(TiO_2(m,n))=2(m+1)^2\left(\frac{91mn^3}{3}+\frac{21mn^2}{2}+\frac{65n^3}{3}-\frac{353mn}{6}-5n^2-39m-\frac{394n}{6}-39\right)$$

Proof. Consider the Titania Planar Nanotubes $TiO_2(m,n)$ for all $m,n\in\mathbb{N}$ with $12(m+1)(\frac{1}{2}n)+4(m+1)=6mn+4m+6n+4=2(3n+2)(m+1)$ vertices/atoms bonds ($|V(TiO_2(m,n))|$) and $10mn+6m+8n+4$ edges/Chemical bonds ($|E(TiO_2(m,n))|$) where $6\left(\frac{n}{2}\right)+2+4(m-1)\left(\frac{n}{2}\right)+0+7+6\left(\frac{n}{2}-1\right)+1=2mn+4n+4$ vertices have degree two, $2\left(\frac{n}{2}\right)+2\left(\frac{n}{2}\right)=2n$ vertices have degree four, $2(m)\left(\frac{n}{2}\right)=2mn$ vertices have degree five and there are $3+2\left(\frac{n}{2}-1\right)+1+5(m-1)+4(m-1)\left(\frac{n}{2}-1\right)+3(m-1)+2\left(\frac{n}{2}+1\right)=2mn+4m$ vertices with degree 3.

Here by using the Cut Method and Orthogonal Cuts of the Titania Nanotubes $TiO_2(m,n)$, we can determine all edge cuts (quasi-orthogonal) of the Titania Nanotubes $TiO_2(m,n)$ in **Table 1** and **Fig. 1.** The edge cut $C(e)$ is an orthogonal cut, such that the set of all edges $f\in E(G)$ are strongly co-distant to e ($C(e):=\{f\in E(G)|f$ *is co-distant with* $e\}$). Also, for further research and study of the cut method and orthogonal cuts in some classes of chemical graphs, see [31, 32]. Some applications of the cut method include the Wiener, hyper-Wiener, weighted Wiener, Wiener-type, Szeged indices and classes of chemical graphs such as trees, Benzenoid graphs and phenylenes.

Now by using the Cut Method and finding Orthogonal Cuts, we can compute the quantities of $n_u(e|TiO_2(m,n))$ and $n_v(e|TiO_2(m,n))$, $\forall e\in E\ (TiO_2(m,n))$, which are the number of vertices in two sub-graphs $TiO_2(m,n)-C(e)$. In case the Titania Nanotubes $TiO_2(m,n)$ $\forall e=uv\in E(TiO_2(m,n))$, we denote $n_u(e|TiO_2(m,n))$ as the number of vertices in the left component of $TiO_2(m,n)-C(e)$ and alternatively $n_v(e|TiO_2(m,n))$ as the number of vertices in the right component of $TiO_2(m,n)-C(e)$, since all edges in $TiO_2(m,n)$ Nanotubes sheets are oblique or horizontal.

Thus, by according to the structure of the Titania Nanotubes $TiO_2(m,n)$ for all integer numbers $m,n>1$, we have following results:

For the edge $e_1=u_1v_1$ that belong to the first square of $TiO_2(m,n)$ Nanotubes (in the first column and row), we see that

$$n_{u1}(e_1|TiO_2(m,n))=2(m+1)$$

and

$$n_{v1}(e_2|TiO_2(m,n))=6mn+4m+6n+4-2(m+1)=6mn+2m+6n+2.$$

For the edge $e_2=u_2v_2$:

$$n_{u2}(e_2|TiO_2(m,n))=3\times 2(m+1)+1\times 2(m+1)=8(m+1)$$

and

$$n_{v2}(e_2|TiO_2(m,n))=6mn+4m+6n+4-8(m+1)=6mn-4m+6n-4.$$

For the edge $e_{n+1}=u_{n+1}v_{n+1}$:

$$n_{u\,n+1}(e_{n+1}|TiO_2(m,n))=(3n+1)\times 2(m+1)$$

and

$$n_{v\,n+1}(e_{n+1}|TiO_2(m,n))=6mn+4m+6n+4-(6mn+6n+2m+2)=2(m+1).$$

Thus, by a simple induction for $i=1,2,\ldots,n;$ we can see that for the edge $e_i=u_iv_i$:

$$n_{ui}(e_i|TiO_2(m,n))=2(m+1)\times(3(i-1)+1)$$

and

$$n_{vi}(e_i|TiO_2(m,n))=6mn+4m+6n+4-(6mi+6i-4m-4)$$
$$=6m(n-i)+6(n-i)+8(m+1)$$
$$=6(m+1)(n-i)+8(m+1)$$
$$=2(m+1)(3(n-i)+4).$$

Let the edge $f_1=u_1v_1\in E(TiO_2(m,n))$ be the first oblique edge in the first square of $TiO_2(m,n)$ Nanotubes (in the first column and row), we see that

$$n_{u1}(f_1|TiO_2(m,n))=m+1$$

and

$$n_{v1}(f_1|TiO_2(m,n))=6mn+4m+6n+4-(m+1)$$
$$=6mn+3m+6n+3$$
$$=6n(m+1)+3(m+1)$$
$$=(6n+3)(m+1).$$

For the edge $f_2=u_2v_2$:

$$n_{u2}(f_2|TiO_2(m,n))=(m+1)+3\times 2(m+1)=7(m+1)$$

and

$$n_{v2}(f_2|TiO_2(m,n))=6mn+4m+6n+4-7(m+1)=6n(m+1)-3(m+1)=(6n-3)(m+1).$$

For the edge $f_{(n+1)}=u\,v$:

$$n_{u(n+1)}(f_{(n+1)}|TiO_2(m,n))=(m+1)+3n\times 2(m+1)=(6n+1)(m+1)$$

and

$$n_{v(n+1)}(f_{(n+1)}|TiO_2(m,n))=(6n+4)(m+1)-(6n+1)(m+1)=3(m+1).$$

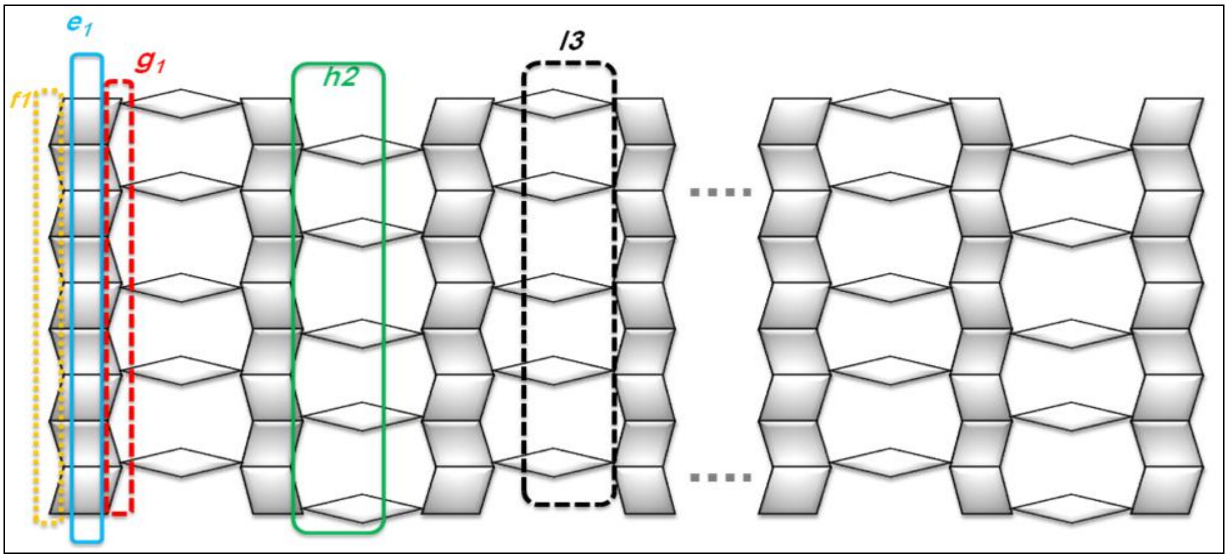

FIG. 2: CATEGORIES FOR EDGES OF THE TITANIA CARBON NANOTUBES $TiO_2(m,n)$.

Therefore, by a simple induction for $j=1,2,\ldots,n+1$; we can see that

For the edge $f_j=u_jv_j$:

$$n_{uj}(f_j|TjO_2(m,n))=3(j-1)\times 2(m+1)+(m+1)=(m+1)(6j-5)$$

and

$$n_{vj}(f_j|TjO_2(m,n))=(6n+4)(m+1)-(m+1)(6j-5)$$
$$=(m+1)(6n-6j+9)$$
$$=3(m+1)(2n+3-2j).$$

Let the edge $g_1=u_1v_1\in E(TiO_2(m,n))$ be the second oblique edge in the first square of $TiO_2(m,n)$ Nanotubes (in the first column and row), so we have

$$n_{u1}(g_1|TiO_2(m,n))=2(m+1)+(m+1)$$

and

$$n_{v1}(g_1|TiO_2(m,n))=(6n+4)(m+1)-3(m+1)=(6n+1)(m+1)$$

For $g_2=u_2v_2$:

$$n_{u2}(g_2|TiO_2(m,n))=3\times 2(m+1)+2(m+1)+(m+1)=9(m+1)$$

and

$$n_{v2}(g_2|TiO_2(m,n))=(6n+4)(m+1)-9(m+1)=(6n-5)(m+1)$$

For $g_{n+1}=u_{n+1}v_{n+1}$:

$$n_{un+1}(g_{n+1}|TiO_2(m,n))=3n\times 2(m+1)+2(m+1)+(m+1)=(6n+3)(m+1)$$

and

$$n_{vn+1}(g_{n+1}|TiO_2(m,n))=(6n+4)(m+1)-(6n+3)(m+1)=(m+1).$$

And these imply that $\forall j=1,2,\dots,n+1$

$$n_{uj}(g_j|TjO_2(m,n))=3j\times 2(m+1)+3(m+1)=(m+1)(6j+3)$$

and

$$n_{vj}(g_j|TjO_2(m,n))=(6n+4)(m+1)-(m+1)(6j+3)=(m+1)(6n-6j+1).$$

Finally, let $h_1=u_1v_1$ & $l_2=u_2v_2\in E(TiO_2(m,n))$ be the first and second oblique edges in the second square of the first row (or the first square in the second column) of $TiO_2(m,n)$ Nanotubes, then

$$n_{u1}(h_1|TiO_2(m,n))=2\times 2(m+1)$$

and

$$n_{u2}(l_2|TiO_2(m,n))=3\times 2(m+1)$$

$$n_{v1}(h_1|TiO_2(m,n))=(6n+4)(m+1)-2(m+1)=(6n+2)(m+1)$$

and

$$n_{v2}(l_2|TiO_2(m,n))=(6n+1)(m+1)$$

And by a simple induction on $\forall i=1,2,\dots,n;$ for the edges $h_i=u_iv_i$ and $l_i=a_ib_i$ we have

$$n_{ui}(h_i|TiO_2(m,n))=3(i-1)\times 2(m+1)+2\times 2(m+1)=2(m+1)(3i-1)$$

and

$$\begin{aligned}n_{vi}(h_i|TiO_2(m,n))&=(6n+4)(m+1)-2(m+1)(3i-1)\\&=(m+1)(6n-6i+6)\\&=6(m+1)(n+1-i).\end{aligned}$$

$$n_{ai}(l_i|TiO_2(m,n))=3(i-1)\times 2(m+1)+3\times 2(m+1)=6i(m+1)$$

and

$$\begin{aligned}n_{bi}(l_i|TiO_2(m,n))&=(6n+4)(m+1)-6i(m+1)\\&=(m+1)(6n-6i+4)\\&=3(m+1)(3n+2-2i).\end{aligned}$$

On the other hands, by according to **Fig. 2,** we can see that the size of all orthogonal cuts for these edge categories in the Titania Nanotubes $TiO_2(m,n)$ are equal to ($\forall i=1,2,\dots,n+1$):

$$|C(e_i)|=|C(h_i)|=|C(l_i)|=2(m+1)$$

And

$$|C(f_i)|=|C(g_i)|=2m+1.$$

Here by above mentions results of $n_u(e|TiO_2(m,n))$ and $n_v(e|TiO_2(m,n))$ ($\forall e\in E(TiO_2(m,n))$, $m,n\in\mathbb{N}-\{1\}$) and according to **Fig. 2**, we will have following computations for the vertex PI, Szeged indices of Titania Carbon Nanotubes $TiO_2(m,n)$.

$$Sz_v(TiO_2(m,n)) = \sum_{e=uv\in E(G)} \left(n_u(e|G)\times n_v(e|G)\right)$$

$$= \sum_{\substack{e_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\dots,n+1}} |C(e_i)|\left(n_u(e_i|TiO_2(m,n))\times n_v(e_i|TiO_2(m,n))\right)$$

$$+ \sum_{\substack{f_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\dots,n+1}} |C(f_i)|\times n_u(f_i|TiO_2(m,n))n_v(f_i|TiO_2(m,n))$$

$$+ \sum_{\substack{g_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\dots,n+1}} |C(g_i)|\times n_u(g_i|TiO_2(m,n))n_v(g_i|TiO_2(m,n))$$

$$+ \sum_{\substack{h_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\dots,n}} |C(h_i)|\times n_u(h_i|TiO_2(m,n))n_v(h_i|TiO_2(m,n))$$

$$+ \sum_{\substack{l_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\dots,n}} |C(l_i)|\times n_u(l_i|TiO_2(m,n))n_v(l_i|TiO_2(m,n))$$

$$= \sum_{i=1}^{n+1} 2(m+1)\left(2(m+1)(3(i-1)+1)\times 2(m+1)(3(n-i)+4)\right)$$

$$+ \sum_{i=1}^{n+1} 2(m+1)\left((m+1)(6i-5)\times 3(m+1)(2n+3-2i)\right)$$

$$+ \sum_{i=1}^{n+1} 2(m+1)\left((m+1)(6i+3)\times (m+1)(6n-6i+1)\right)$$

$$+ \sum_{i=1}^{n} (2m+1)\left(2(m+1)(3i-1)\times (m+1)(n+1-i)\right)$$

$$+ \sum_{i=1}^{n} (2m+1)\left(6i(m+1)\times 3(m+1)(3n+2-2i)\right)$$

$$= 8(m+1)^3 \sum_{i=1}^{n+1} (3(i-1)+1)(3(n-i)+4)$$

$$+6(m+1)^3 \sum_{i=1}^{n+1} (6i-5)(2n+3-2i)$$

$$+2(m+1)^3 \sum_{i=1}^{n+1} (6i+3)(6n-6i+1)$$

$$+2(2m+1)(m+1)^2 \sum_{i=1}^{n} (3i-1)(n+1-i)$$

$$+18(2m+1)(m+1)^2 \sum_{i=1}^{n} i(3n+2)-2i^2$$

$$= 2(m+1)^2 [4(m+1)\sum_{i=1}^{n+1}\left(-6i^2+(9n+10)i-2(3n+2)\right)$$

$$+3(m+1)\sum_{i=1}^{n+1}\left(-12i^2+(12n+25)i-5(2n+3)\right)$$

$$+(m+1)\sum_{i=1}^{n+1}\left(-18i^2+6(n-2)i+3(6n+1)\right)$$

$$+(2m+1)\sum_{i=1}^{n}\left(-i^2+(3n+4)i-(n+1)\right)$$

$$+9(2m+1)\sum_{i=1}^{n}\left(-2i^2+(3n+2)i\right)]$$

$$=2(m+1)^2\begin{bmatrix}(m+1)\sum_{i=1}^{n+1}\left(-78i^2+(78n+103)i-(72n+64)\right)\\+(2m+1)\sum_{i=1}^{n}\left(-19i^2+(30n+22)i-(n+1)\right)\end{bmatrix}$$

$$=2(m+1)^2\begin{bmatrix}(m+1)\sum_{i=1}^{n}\left(-78i^2+(78n+103)i-(72n+64)\right)-(47n+39)\\+(2m+1)\sum_{i=1}^{n}\left(-19i^2+(30n+22)i-(n+1)\right)\end{bmatrix}$$

$$=2(m+1)^2[(m+1)\left[\left(-78\left(\frac{n^3}{3}+\frac{n^2}{2}+\frac{n}{6}\right)+(78n+103)\left(\frac{n^2}{2}+\frac{n}{2}\right)-n(72n+64)\right)-(47n+39)\right]$$

$$+(2m+1)\left(-19\left(\frac{n^3}{3}+\frac{n^2}{2}+\frac{n}{6}\right)+(30n+22)\left(\frac{n^2}{2}+\frac{n}{2}\right)-n(n+1)\right)]$$

$$=2(m+1)^2\left[(m+1)\left(-\frac{78n^3}{3}-\frac{78n^2}{2}-\frac{78n}{6}+\frac{78n^3}{2}+\frac{181n^2}{2}+\frac{103n}{2}-72n^2-64n-47n-39\right)\right.$$

$$\left.+(2m+1)\left(-\frac{19n^3}{3}-\frac{19n^2}{2}-\frac{19n}{6}+15n^3+26n^2+11n-n^2-n\right)\right]$$

$$=2(m+1)^2\left[(m+1)\left(13n^3-\frac{41n^2}{2}-\frac{145n}{2}-39\right)+(2m+1)\left(\frac{26n^3}{3}+\frac{31n^2}{2}+\frac{41n}{6}\right)\right]$$

$$=2(m+1)^2\left(\frac{91mn^3}{3}+\frac{21mn^2}{2}+\frac{65n^3}{3}-\frac{353mn}{6}-5n^2-39m-\frac{394n}{6}-39\right)$$

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