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Computing Cluj Index of $TUC_4C_8(S)$ Nanotube

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Abstract. The Cluj index is a topological index that is defined as: $[UM]_{ij} = max|v_{i,j,p_k}|$; $k = 1, 2, ...$ where,

$$v_{i,j,p_k} = \{v|v \in V(G); d_{iv} < d_{jv}; (i,v)_h \cap p_k = i; p_k \in D(G) or \Delta(G); h,k = 1,2,..\}$$

In this paper, we find an exact formula for the Cluj index of $TUC_4C_8(S)$ nanotubes.

1 Introduction

Mathematical calculations are absolutely necessary to explore the important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structures using mathematical methods without necessarily referring to the quantum mechanics. Chemical graph theory is an important tool for studying the molecular structures. This theory had an important effect on the development of chemical sciences. A topological index is a real number related to a molecular graph. It must be a structural invariant. It does not depend on either the labeling or the pictorial representation of a graph. Several indices have been so far defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecular structures. The Wiener Index is the first topological index to be used in chemistry([1–5, 17, 18]).

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It was introduced in 1974 by Harlod Wiener as" the path number for characterization of alkanes". The unsymmetric Cluj matrix [6], UCJ, has been proposed by Diudea [7]. It is defined by using either the distance or the detour concept. The non-diagonal entries; $[UM]_{ij}$; $M = CJD$(Cluj-Distance) or $CJ\Delta$(Cluj-Detour), are defined as:

$$[UM]_{ij} = max|v_{i,j,p_k}| \; k = 1, 2, \ldots$$

$$v_{i,j,p_k} = \{v|v \in V(G); d_{iv} < d_{jv}; (i,v)_h \cap p_k = i; p_k \in D(G) or \Delta(G); h, k = 1, 2, ..\} \; .$$

where, $|v_{i,j,p_k}|$ is the cardinality of the set v_{i,j,p_k}; which is taken as the maximum overall paths $p_k = (i,j)_k$. $D(G)$ and $\Delta(G)$ are the set of distances (i.e, geodesics) and detours (i.e, elongations), respectively. The set v_{i,j,p_k} consists of vertices v lying closer to the vertex i (condition $d_{iv} < d_{jv}$). This variant of Cluj matrices is called at least one of the pathes $(v,i)_h$ must be external with respect to the path $(i,j)_k : (i,v)_h \cap p_k = i$. In cycle-containing structures; more one than path $(i,j)_k$ may exist; thus supplying various sets of v_{i,j,p_k}. By definition, the (i,j)-entry in the Cluj matrices are square arrays of dimension $N \times N$, usually unsymmetric, where v_{i,j,p_k} is the set of disconnected vertices. This fact is undesirable when molecular graph (which are always connected graphs) are investigated. If v_{i,j,p_k} real (connected) chemical fragments are wanted, the Cluj fragmental matrices are defined. In this version; the sets of v_{i,j,p_k} defined as:

$$v_{i,j,p_k} = \{v|v \in V(G_p); G_p = G - p_k; d_{iv}(G_p) < d_{jv}(G_p); p_k \in D(G) or \Delta(G)\}$$

where $d_{iv}(G_p)$ and $d_{jv}(G_p)$ are the topological distances between the vertex v and the vertices i and j, respectively in the spanning subgraph G_p resulted by cutting the path $p_k = (i,j)_k$ (except its endpoints) from G. Now the set of v_{i,j,p_k} consists of vertices lying closer to the vertex i in G_p. This version is called all pathes external to the path $(i,j)_k$; by reason that all paths $(i,v)_h; h = 1, 2, ...$ are external with respect to p_k, since the last path was already cut off. The diagonal entries are zero.

The cluj indices are calculated ([7–16]) as half-sum of the entries in a Cluj symmetric matrix; M, $M = CJD, CJ\Delta, CFD, CF\Delta$

$$IE(M) = \frac{1}{2} \sum_i \sum_j [M]_{ij} [A]_{ij} \tag{1}$$

$$IP(M) = \frac{1}{2} \sum_i \sum_j [M]_{ij} \tag{2}$$

or from an unsymmetric Cluj matrix, by:

$$IE2(UM) = \frac{1}{2}\sum_i \sum_j [UM]_{ij}[UM]_{ij}[A]_{ij} \tag{3}$$

$$IP2(UM) = \frac{1}{2}\sum_i \sum_j [UM]_{ij}[UM]_{ij} \tag{4}$$

The number defined on edge, IE, is an index, while the number defined on path; IP, is a hyper-index. Note that the operators, IE and IP, as well as the operators,IE2 and IP2, may be applied to both symmetric and unsymmetric matrices. When the last two operators are calculated on a symmetric matrix, the terms of sum represent the squared entries in that matrix. This is the reason for the number 2 in the symbol of these operators. It is obvious that $IE(M) = IE2(UM)$ and $IP(M) = IP2(UM)$ with the condition that $M = (UM)(UM)^T$, where, $(UM)^T$ is the transpose of the unsymmetric matrix, UM.

2 Construction of $TUC_4C_8(S)$ nanotube

$TUC_4C_8(S)$ nanotube is made of octagonal and tetrahedron. In $TUC4C8(S)[p, q]$; the first letter in the bracket is the number of octagons in the first row, while q denotes the number of octagons in the first column.

Remark 1. $TUC_4C_8(S)$ has horizontal and vertical symmetry lines (see Figure 1).

Remark 2. $TUC_4C_8(S)$ has $4p\ q$ vertices (see Figure 1).

3 Results and discussion

In this section, we obtain an exact formula for the Cluj index of $TUC_4C_8(S)$ on edge.

By using (1), we have the following formula:

$$IE(CJD) = \frac{1}{2}\sum_i \sum_j [CJD]_{ij}[A]_{ij} \tag{5}$$

Definition 1. The sum of entries in the i^{th} row of $[CJD]_{ij}[A]_{ij}$ is called as the value of the i^{th} vertex , which is denoted by v_i. So, we obtain the value of all vertices by $"Topo - Cluj"$. Now we compute the Cluj index of $TUC_4C_8(S)[p, q]$ by relation (5).

Let G be the graph of $TUC_4C_8(S)[p, q]$ (see Figure 1). In this graph, all of vertices have degree two or three. In the following lemmas, we will obtain the values of all vertices of degree two and three, separately.

Lemma 1. The total values of all vertices, which have degree two in the $TUC_4C_8(S)[p,q]$

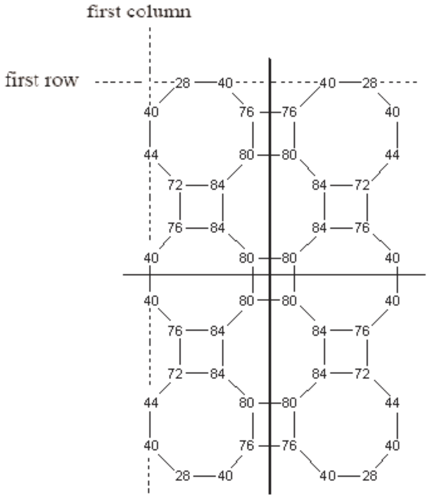

Figure 1: $TUC_4C_8(S)[2,3]$

are equal to:

$$\frac{32}{3}p^3 + \frac{32}{3}p^2q + \frac{16}{3}p + 16p\,q + 32q^2 \tag{6}$$

Proof. The lemma is approved by using of Table 1 and (2) and relation (5).

Table 1, is the table of all vertices values, which have degree two at the first row.

Table 1: The values of vertices of degree two at the first row

$q \rightarrow$ / $p \downarrow$		1	2	3	4	5
1	*valuation*	8	12	16	20	24
	number	4	4	4	4	4
2	*valuation*		$24, 28$	$28, 40$	$32, 52$	$36, 64$
	number		$4, 4$	$4, 4$	$4, 4$	$4, 4$
3	*valuation*			$48, 52, 64$	$52, 64, 84$	$57, 76, 104$
	number			$4, 4, 4$	$4, 4, 4$	$4, 4, 4$
4	*valuation*				$80, 84, 96, 116$	$84, 96, 116, 144$
	number				$4, 4, 4, 4$	$4, 4, 4, 4$
5	*valuation*					$120, 124, 136, 156, 184$
	number					$4, 4, 4, 4, 4$

At first, we obtain the exact formula for the total values of all vertices in the first row (when octagons joint with each other there are vertices of degree three at the first row).

The smallest value of vertices in $TUC_4C_8(S)[p,q]$ is equal to $4(q+p^2)+8pq$. The next values of vertices follow the formula below:

$$4(p-k)(2q-(p+k))\ ; \quad k=1,...,p-1$$

The number of vertices for these values is equal to 4.

Then we have:

$$4\times(4(q+p^2)+8pq)+4\times\left(\sum_{k=1}^{p-1}\left(4(q+p^2)+4((p-k)(2q-(p+k)))+8pq\right)\right)$$
$$=8p^2+48p^2\ q+\frac{16}{3}p^3+\frac{8}{3}p \tag{7}$$

Next, we obtain the exact formula for the total values of all vertices in the first column (there are vertices of degree two at the first column). Table (2) shows the values of all vertices which have degree two at the first column.

Table 2: The values of vertices of degree two at the first column

$q\rightarrow$ / $p\downarrow$		1	2	3	4	5
1	*valuation*	8	16	24	32	40
	number	4	8	12	16	20
2	*valuation*		24, 28	40, 44	56, 60	72, 76
	number		4, 4	8, 4	12, 4	16, 4
3	*valuation*			48, 52, 64	72, 76, 88	108, 112, 124
	number			4, 4, 4	8, 4, 4	12, 4, 4
4	*valuation*				80, 84, 96, 116	112, 116, 128, 148
	number				4, 4, 4, 4	8, 4, 4, 4
5	*valuation*					120, 124, 136, 156, 184
	number					4, 4, 4, 4, 4

The smallest value of these vertices in $TUC_4C_8(S)[p,q]$ is equal to $4p(2q-(p-1))$. The next values of vertices is equal to $k^2\ ,\quad k=1,...,p-1$.

The numbers of vertices for the above values is equal to:

$$\begin{cases} 4(q-(p-1)) & k=0 \\ 4 & k\neq 0\ . \end{cases}$$

So, we have:

$$4(q-(p-1))\times 4p(2q-(p-1))+4\times\sum_{k=1}^{p-1}(4p(2q-(p-1))+4k^2)$$
$$=32q^2-16p^2q+16qp-8p^2+\frac{16}{3}p^3+\frac{8}{3}p \tag{8}$$

Finally, we obtain the total values of all vertices of degree two by adding up (7) and (8).

Hence, the total values of all vertices which have degree two in the $TUC_4C_8(S)[p,q]$ are equal to:

$$\frac{32}{3}p^3+\frac{32}{3}p^2q+\frac{16}{3}p+16p\ q+32q^2 \tag{9}$$

Lemma 2. The total values of all vertices which have degree three in the $TUC_4C_8(S)[p,q]$ are equal to:

$$-16q\ p^2-\frac{16}{3}p+96q^2\ p^2-48q^2\ p-16q\ p-\frac{32}{3}p^3. \tag{10}$$

Proof. The lemma is approved by using of Table 3 and relation (5).

Table 3 shows the values of all vertices which have degree three.

Table 3: The valuaes of vertices of degree three

$q\rightarrow$ / $p\downarrow$	*column number*	1	2	3	4	5
1	2	0	28	40	52	64
	number	0	4	8	12	16
2	2		52	72, 76	92, 96	112, 116
	number		4	4, 4	4, 4	4, 4
	4		52, 56	76, 80	100, 104	124, 128
	number		4, 4	4, 8	4, 12	4, 16
	3		56	84	112	140
	number		4	8	12	16
3	2			104, 116	132, 144, 148	160, 172, 176
	number			4, 4	4 , 4 , 4	4 , 4 , 8
	4			104, 116, 120	136, 148, 152	168, 180, 184
	number			4 , 4 , 4	4 , 4 , 8	4 , 4 , 12
	6			116, 120	152, 156	188, 192
	number			4, 4	4, 8	4, 12
	5			116, 120, 124	156, 160, 164	196, 200, 204
	number			4 , 4 , 4	4 , 8 , 4	4 , 12 , 4
	3			120, 124	164, 168	208, 212
	number			4, 4	8, 4	12, 4
4	2				172, 192, 204	208, 228, 240, 244
	number				4 , 4 , 4	4 , 4 , 4 , 4
	4				172, 192, 204, 208	212, 232, 244, 248
	number				4 , 4 , 4 , 4	4 , 4 , 4 , 8
	6				192, 204, 208	236, 248, 252
	number				4 , 4 , 4	4 , 4 , 8
	8				192, 204, 208, 212	240, 252, 256, 260
	number				4 , 4 , 4 , 4	4 , 4 , 8 , 4
	7				204, 208, 212	256, 260, 264
	number				4 , 4 , 4	4 , 8 , 4
	5				204, 208, 212, 224	260, 264, 268, 280
	number				4 , 4 , 4 , 4	4 , 8 , 4 , 4
	3				208, 212, 224	268, 272, 284
	number				4 , 4 , 4	8 , 4 , 4

We can obtain the values of vertices of degree three by the following method:

1-The values of even columns are arranged from top to bottom.

2-The values of odd columns are arranged from bottom to top.

3-From top, we put the values of two columns in one brace like the sample below:

$$\begin{aligned} k=p-1 &= \begin{cases} 2 \\ 4 \end{cases} \\ &\vdots \\ k=1 &= \begin{cases} 7 \\ 5 \end{cases} \\ k=0 &= \{3 \end{aligned}$$

Remark 3. The values of the third column are always put in one brace.

During this process; we observe that one of the sequences in one brace is shorter than the other sequence except for $k=0$ (because it has just one value sequence) and $k=p-1$ that has two value sequences with same length except for $p=q$ mode. The smallest values of vertices in the second column in $k=p-1$ brace is equal to $4((2p+1)q+(2p-1))$. The smallest values of other columns is equal to:

$$\begin{cases} 4((2p+1)\ q+(2p-1)+((p-1)^2-k^2)+(q-p)\ (2p-(2k+2))) \\ k=0,...,p-1 \qquad \text{short sequence} \\ \\ 4((2p+1)\ q+(2p-1)+((p-1)^2-k^2)+(q-p)\ (2p-(2k+1))) \\ k=1,...,p-1 \qquad \text{long sequence} \end{cases}$$

Distance of the next values from the smallest one in each sequence are equal to $j(2k-j)$, $j=0,...,k-1$ and the rest of values are equal to:

$$(k^2-1)+i(i-2)$$
$$i=\begin{cases} 1,..,p-(k+1) & k=0,...,p-2 \\ 1 & k=p-1. \end{cases}$$

Therefore, we have:

$$\begin{cases} 4((2p+1)\ q+(2p-1)+((p-1)^2-k^2)+(q-p)\ (2p-(2k+2))+j(2k-j) \\ k=0,...,p-1 \quad j=1,...,k-1 \qquad \text{short sequence} \\ 4((2p+1)\ q+(2p-1)+((p-1)^2-k^2)+(q-p)\ (2p-(2k+1))+j(2k-j)) \\ k=1,...,p-1 \quad j=1,...,k-1 \qquad \text{long sequence} \end{cases}$$

For the rest of values, we have:

$$\begin{cases} 4((2p+1)q+(2p-1)+((p-1)^2-k^2)+(q-p)(2p-(2k+2))+(k^2-1)+(i(i-2)+2)) \\ i=\begin{cases} 1,..,p-(k+1) & k=0,...,p-2 \\ 1 & k=p-1. \end{cases} \qquad \text{short sequence} \\ \\ 4((2p+1)\ q+(2p-1)+((p-1)^2-k^2)+(q-p)\ (2p-(2k+1))+(k^2-1)+(i(i-2)+2)) \\ k=1,...,p-1 \quad i=1,...,p-1 \qquad \text{long sequence} \end{cases}$$

The numbers of vertices for the above values are equal to:
1-For $i=1$, there are 4(q-(p-1)) vertices.

2-For short sequence, when $k=p-1$ and $i=1$, there are $4(q-p)$ vertices.

3- Otherwise, there are 4 vertices.

At last,

$$\begin{aligned}&4\Bigg(\sum_{k=0}^{p-1}\sum_{j=0}^{k-1}(4((2p+1)q+(2p-1))+((p-1)^2-k^2)\\&+(q-p)(2p-(2k+2))+j(2k-j))\Bigg)\\&=\frac{64}{3}qp^3-24qp^2+\frac{8}{3}qp-\frac{28}{3}p^2+\frac{4}{3}p^4+8p^3\end{aligned}\tag{11}$$

$$\begin{aligned}&4\Bigg(\sum_{k=1}^{p-1}\sum_{j=0}^{k-1}(4((2p+1)q+(2p-1))+((p-1)^2-k^2)\\&+(q-p)(2p-(2k+1))+j(2k-j))\Bigg)\\&=\frac{64}{3}qp^3-16qp^2-\frac{16}{3}qp-\frac{4}{3}p^2+\frac{4}{3}p^4\end{aligned}\tag{12}$$

$$\begin{aligned}&4\Bigg(\sum_{k=0}^{p-2}\sum_{i=2}^{p-(k+1)}(4((2p+1)q+(2p-1))+((p-1)^2-k^2)\\&+(q-p)(2p-(2k+1))+(k^2-1)+i(i-2)+2)\Bigg)\\&=-16+\frac{40}{3}p-16q-\frac{104}{3}qp+\frac{4}{3}p^2-\frac{4}{3}p^4+\frac{8}{3}p^3+\frac{80}{3}qp^3+24qp^2\end{aligned}\tag{13}$$

$$\begin{aligned}&4(q-(p-1))\Bigg(\sum_{k=0}^{p-2}(4((2p+1)q+(2p-1))+((p-1)^2-k^2)\\&+(q-p)(2p-(2k+2))+(k^2))\Bigg)=-16(-q+p-1)(p-1)q(3p+1)\end{aligned}\tag{14}$$

$$(4(q-p)(4((2p+1)q+(2p-1))+(p-1)^2))=-16(-q+p)(2qp+q+p^2)\tag{15}$$

$$\begin{aligned}&4\Bigg(\sum_{k=1}^{p-1}\sum_{i=2}^{p-k}(4((2p+1)q+(2p-1))+((p-1)^2-k^2)\\&+(q-p)(2p-(2k+1))+(k^2-1)+i(i-2)+2)\Bigg)\\&=-\frac{160}{3}qp+\frac{80}{3}qp^3-\frac{4}{3}p^4-\frac{68}{3}p^2-80qp^2+\frac{40}{3}p+\frac{32}{3}p^3\end{aligned}\tag{16}$$

The total values of all vertices, which have degree three in the $TUC_4C_8(S)[p,q]$ are obtained by adding up (11),(12),(13),(14),(15) and (16). So lemma is approved as:

$$-16q\ p^2 - \frac{16}{3}p + 96q^2\ p^2 - 48q^2\ p - 16q\ p - \frac{32}{3}p^3.$$

The main result of this section is the following theorem.

Theorem. The Cluj index of $TUC_4C_8(S)[p,q]$ is equal to:

$$IE(CJD) = 16p^2q + 32q^2 + 96q^2p^2 - 48q^2p^2.$$

Proof. The theorem is approved by the above lemmas and relation (5).

Remark 4. If the figure of $TUC_4C_8(S)$[p,q] rotates 90 degree, there will be no difference in the values of all vertices. Hence, Cluj index of $TUC_4C_8(S)$[p,q] is equal to Cluj index of $TUC_4C_8(S)$[q,p].

Example. For p=2 and q=2, cluj index of $TUC_4C_8(S)[p,q]$ is equal to 704.

4 Conclusion

One of the famous topological indices is Cluj index. In this paper we could obtain the exact formula for the Cluj index of $TUC_4C_8(S)[p,q]$ nanotube.

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