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Research article

Non-self-centrality number of some molecular graphs

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Abstract: Let $\mathcal{G}$ be a molecular graph, the eccentricity $e(w)$ of the vertex w in $\mathcal{G}$ is the maximum distance of w from any other vertex of $\mathcal{G}$. The non-self-centrality number (NSC) of a graph $\mathcal{G}$ is defined by $N(\mathcal{G}) = \sum_{w \neq z} |e(w) - e(z)|$, where summation goes over all the unordered pairs of vertices of $\mathcal{G}$. We determine non-self-centrality number of TUC_4C_8 and V-phenylenic nanotubes in this paper.

Keywords: non-self-centrality number; topological indices; eccentricity; molecular graphs; non-self-centered graphs; NSC number
Mathematics Subject Classification: 05C12

1. Introduction

Let $\mathcal{G}$ be a connected graph with vertex set $\mathcal{V}(\mathcal{G})$ and edge set $\mathcal{E}(\mathcal{G})$. Two adjacent vertices $w, z \in \mathcal{V}(\mathcal{G})$ are denoted by wz (or zw). The order (resp. size) of $\mathcal{G}$ is $|\mathcal{V}(\mathcal{G})|$ (resp. $|\mathcal{E}(\mathcal{G})|$). The distance between w and z in $\mathcal{G}$ is the length of a shortest path connecting w and z and is denoted by $d_{\mathcal{G}}(w, z)$. For a vertex $w \in \mathcal{V}(\mathcal{G})$, its eccentricity is defined as $e_{\mathcal{G}}(w) = \max\{d_{\mathcal{G}}(w, z) \mid z \in \mathcal{V}(\mathcal{G})\}$. For convenience, we can denote the eccentricity of $w \in \mathcal{G}$ by $e(w)$ if no ambiguity occurs. Furthermore, the minimum eccentricity over all the vertices of a graph $\mathcal{G}$ is called its radius of $\mathcal{G}$ denoted by $r(\mathcal{G})$. Similarly, the maximum eccentricity over all the vertices of a graph $\mathcal{G}$ is called diameter of $\mathcal{G}$ denoted by $d(\mathcal{G})$. A vertex $w \in \mathcal{V}(\mathcal{G})$ is said to be diametrical (resp. central) vertex of $\mathcal{G}$ if $e(w) = d(\mathcal{G})$ (resp. $e(w) = r(\mathcal{G})$). Moreover, the periphery $P(\mathcal{G})$ of a graph $\mathcal{G}$ is defined as

$$P(\mathcal{G}) = \{w \in \mathcal{V}(\mathcal{G}) \mid e(w) = d(\mathcal{G})\}.$$

Whereas, center of a graph $\mathcal{G}$ is the subgraph induced by the central vertices of $\mathcal{G}$. The neighborhood $\mathcal{N}_{\mathcal{G}}(w)$ of a vertex $w \in \mathcal{V}(\mathcal{G})$ is defined as $\mathcal{N}_{\mathcal{G}}(w) = \{z \in \mathcal{V}(\mathcal{G}) \mid wz \in \mathcal{E}(\mathcal{G})\}$. The degree $\deg(w)$ of a vertex w in $\mathcal{G}$ is the number $|\mathcal{N}_{\mathcal{G}}(w)|$. A connected graph is called self-centered if the eccentricities of all the vertices are equal; otherwise, $\mathcal{G}$ is called a non-self-centered graph, shown in Figure 1.

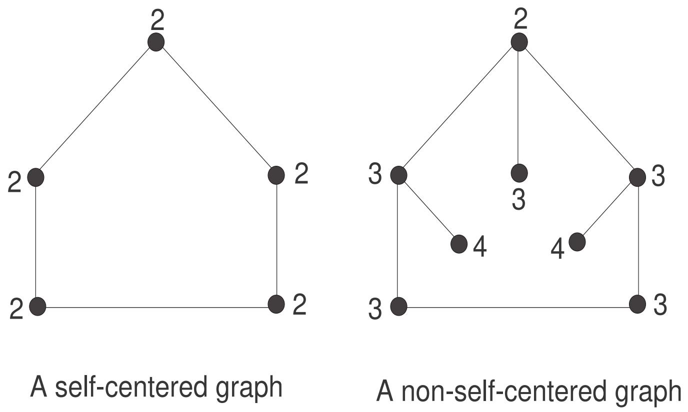

Figure 1. Graphs labeled with vertex eccentricities.

A molecular graph $\mathcal{G}$ represents a chemical compound. A topological index is a numerical parameter of a molecular graph $\mathcal{G}$ which characterizes the properties of $\mathcal{G}$. Topological indices can be divided into many classes; some of them are degree-based, eccentricity-based, and distance-degree-based indices.

Recently, Xu et al. [7] introduced a new graphic invariant for indicating the non-self centrality of the graph more efficiently. This invariant was named as non-self centrality number (henceforth, NSC) of a graph $\mathcal{G}$, which is given by

$$N(\mathcal{G}) \quad = \quad \sum_{w \neq z} |e(w) - e(z)|, \tag{1.1}$$

where sum is over all vertex pair of vertices of a graph $\mathcal{G}$. For non-self-centered graph $\mathcal{G}$, the formula (1.1) was further simplified using the eccentricity sequence of the graph. If the eccentricity e_i appears $l_i \geq 1$ times in $\mathcal{G}$ we write, $e_i^{l_i}$ in short. Let us assume that $e_1 > e_2 > \cdots > e_k$ be the distinct eccentricities of $\mathcal{G}$ with $l_1, l_2, ..., l_k$ be their respective multiplicities. Then the eccentricity sequence is $\zeta(\mathcal{G}) = \{e_1^{l_1}, e_2^{l_2}, \ldots, e_k^{l_k}\}$. Therefore, the NSC number of $\mathcal{G}$ can be written as

$$N(\mathcal{G}) \quad = \quad \sum_{1 \leq i < j \leq k} l_i l_j (e_i - e_j). \tag{1.2}$$

We refer [4] to the readers for some more results on NSC number. By graph structure, we can easily calculate the eccentricities of its vertices. When the eccentricities of vertices of a graph are known, the eccentricity sequence can easily be obtained. Therefore, we will write directly the eccentricity sequences of graphs in this paper.

Ashrafi et al. [3] computed the eccentric-connectivity index of TUC_4C_8 nanotubes and nanotori. Also Kwun et al. [5] computed M-polynomials and topological indices like Zagreb indices of V-phenylenic nanotubes and nanotori. For further details, we refer [1, 2, 6]. Heretofore, NSC number is considered for finite family of graphs [7, 4]. It motivates us to consider NSC number of infinite family of graphs. In this paper, we calculate NSC number of TUC_4C_8 and V-phenylenic nanotubes.

2. V-phenylenic nanotubes

Here we compute the non-self centrality number of V-phenylenic nanotubes. An infinite structure of V-phenylenic nanotubes and nanotori is made by alternating C_4, C_6 and C_8 cycles. The arrangement of C_4, C_6 and C_8 cycles in V-phenylenic structure is such that C_4 ring is attached to two C_6 rings and also each C_4 is attached to two C_8 rings. We will denote the V-phenylenic nanotubes by $G[h, f]$, where f and h are the number of columns and rows, respectively, as shown in the Figures 2 and 3. Consider

$$X = \{z \in \mathcal{V}(G[h, f]) \mid \deg(z) = 2\},$$

and

$$Y = \{z \in \mathcal{V}(G[h, f]) \mid \deg(z) = 3\}.$$

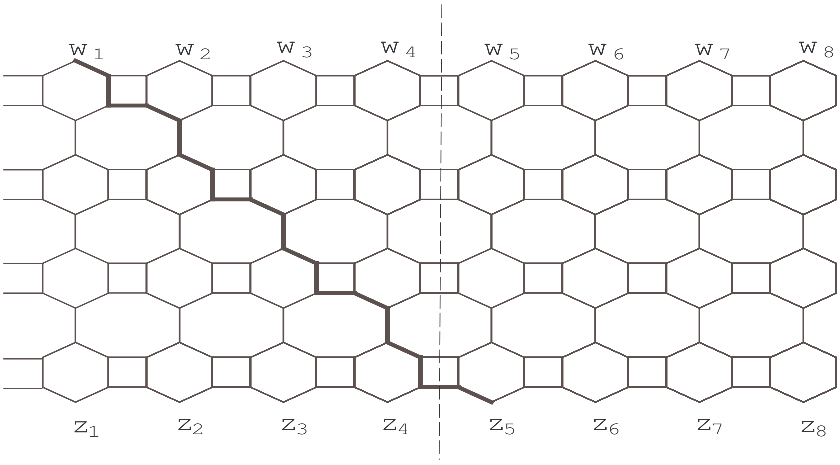

Figure 2. $G[8, 4]$.

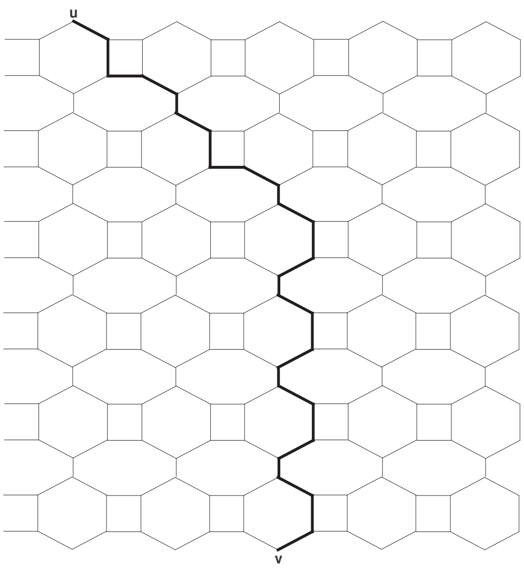

Figure 3. $G[5, 6]$.

Then $|X| = 2h$ and $|Y| = 6hf - 2h$. From the structure of $G[h, f]$, we notice that there are two types of edges given by

$$\mathcal{E}_1 = \{wz \in \mathcal{V}(G[h, f]) \mid \deg(w), \deg(z) = (2, 3)\}$$

and

$$\mathcal{E}_2 = \{wz \in \mathcal{V}(G[h, f]) \mid (\deg(w), \deg(z)) = (3, 3)\}.$$

It is easy to see that $|\mathcal{E}_1| = 4h$ and $|\mathcal{E}_2| = h(9f - 5)$. Hence, $|\mathcal{E}| = |\mathcal{E}_1| + |\mathcal{E}_2| = h(9f - 1)$ is the number of total edges in $G[h, f]$.

Before moving to the main results, it is important to know that structure of V-phenylenic nanotube is symmetric and hence it can be divided into two halves as shown in Figure 2. Whereas, we can also divide the structure into two different classes depending on h and f. When $h < 2f$ we get a vertical structure shown in Figure 3, while we obtain a horizontal structure for $h > 2f$. Now let us begin with the following result:

Lemma 1. For $f \geq 2$ the diameter of $G[h, f]$ is

$$d(G[h, f]) = \begin{cases} \frac{h}{2} + 4f - 1 & h \leq 2f \text{ and } h \text{ is even} \\ \frac{h-3}{2} + 4f & \text{if } h \leq 2f \text{ and } h \text{ is odd} \\ \frac{3h}{2} + 2f - 1 & \text{if } h > 2f \text{ and } h \text{ is even} \\ \frac{3(h-1)}{2} + 2f & \text{if } h > 2f \text{ and } h \text{ is odd.} \end{cases} \tag{2.1}$$

Proof. Let w_i and z_j, $1 \leq i, j \leq h$, be the peripheral vertices in $G[h, f]$, as shown in Figure 2. We can partition $\mathcal{E}(G[h, f])$ into three classes; horizontal, oblique and vertical edges. Now if $h \leq 2f$ and h is an even integer then, to find the diameter we have to find the path's length that connects two vertices of X. Let w_i be the vertex with an eccentric vertex z_j in $G[h, f]$, shown in Figure 2. For $j < (\frac{h}{2} + i)$, length of a shortest w_i, z_j-path contains $2f$ oblique, $(2f - 1)$ vertical and $j - 1$ horizontal edges. Therefore,

$$d_{G[h,f]}(w_i, z_j) = 4f + j - 2.$$

Similarly, for $j = (\frac{h}{2} + i)$, the length of a shortest w_i, z_j-path contains exactly $2f - 1$ vertical, $2f$ oblique and $\frac{h}{2}$ horizontal edges. Therefore,

$$d_{G[h,f]}(w_i, z_j) = \frac{h}{2} + 4f - 1.$$

Now for $j > (\frac{h}{2} + i)$, the length of the shortest w_i, z_j-path contains $2f$ oblique, $(2f - 1)$ vertical and $h - j$ horizontal edges. Therefore,

$$d_{G[h,f]}(w_i, z_j) = 4f + h - j.$$

From the above discussion and Figure 2, it is observed that $d_{G[h,f]}(w_i, z_j) = \frac{h}{2} + 4f - 1$ is the maximum distance. Therefore, $d(G[h, f]) = \frac{h}{2} + 4f - 1$.

Similarly, in case of odd h, we choose w_i and z_j, where $z_j \in X \cup Y$, such that $d_{G[h,f]}(w_i, z_j)$ is maximum. We need $2f$ oblique edges, $2f - 1$ vertical edges and $\frac{h-1}{2}$ horizontal edges to connect w_i and z_j. Hence, the diameter is given by $d(G[h, f]) = \frac{h-3}{2} + 4f$. In similar manner, we can find the diameter of $G[h, f]$ when $h < 2f$.

Theorem 2. For $f \geq 2$, we have

$$N(G[h,f]) = \begin{cases} 2h^2f[3f^2+1] & \text{if } h > 2f-1 \\ & \text{and } h \text{ is even} \\ 6fh^2(f+1)(f-1) & \text{if } h > 2f-1 \\ & \text{and } h \text{ is odd} \\ h^2[6f^3+122f-216] & \text{if } h = 2f-2 \\ & \text{or } h = 2f-1 \\ 4h^2\Big[2f^3+\frac{s}{2}(2f^2-5)\Big] & \text{if } h < 2f-2 \\ & \text{and } f \text{ is even} \\ 4h^2[3f^3-f] & \text{if } h < 2f-2 \\ & \text{and } f \text{ is odd.} \end{cases} \tag{2.2}$$

Proof. We discuss five possible cases:
Case 1: $h > 2f-1$ and h is even.
Here we have

$$\zeta(G[h,f]) \quad = \quad \{e_1^{2h}, e_2^{6h}, \ldots, e_f^{6h}, e_{f+1}^{4h}\}.$$

Using formula (1.2), the NSC number of $G[h,f]$ is given by

$$\begin{aligned} N(G[h,f]) =& [(2h)(4h)+(2h)(4h)(2)+\cdots+ \\ & (2h)(6h)(f)] + [(4h)(4h)+\ldots \\ & +(4h)(6h)(f-1)] + \cdots + [(4h)(6h)]. \end{aligned}$$

After simplification, we get

$$\begin{aligned} N(G[h,f]) &= 18h^2f^2 - 10h^2f + 6h^2f(f-1)(f-2) \\ &= 2h^2f[3f^2+1]. \end{aligned}$$

Case 2: $h > 2f-1$ and h is odd.
In this case, we have

$$\zeta(G[h,f]) \quad = \quad \{e_1^{6h}, e_2^{6h}, \ldots, e_f^{6h}\}.$$

Using (1.2), the NSC number of $T[h,f]$ is given by

$$\begin{aligned} N(G[h,f]) &= 18h^2f^2[(1)(2)+\cdots+(f-2)(f-1) \\ &\quad + f(f-1)] \\ &= 6h^2f(f+1)(f-1). \end{aligned}$$

Case 3: $h \in \{2f-2, 2f-1\}$.
The eccentricity sequence of $G[h,f]$ in this case is given by

$$\zeta(G[h,f]) = \{e_1^{2h}, e_2^{4h}, e_3^{4h}, e_4^{2h}, e_5^{2h}, e_6^{6h}, \ldots, e_{f+2}^{6h}, e_{f+3}^{4h}\}. \tag{2.3}$$

Using formula (1.2), the NSC number of $G[h, f]$ is given by

$$\begin{aligned} N(G[h, f]) =& 2h[4h + 4h\{2\} + 2h\{3\} + 2h\{4\} \\ &+ 6h\{5\} + 6h\{6\} + \cdots + 6h\{f + 1\} \\ &+ 4h\{f + 2\}] + 4h[4h + 2h\{2\} \\ &+ 2h\{3\} + 6h\{4\} + 6h\{5\} + \cdots + 6h\{f\} \\ &+ 4h\{f + 1\}] + 4h[2h + 2h\{2\} \\ &+ 6h\{3\} + 6h\{4\} + \cdots + 6h\{f - 1\} \\ &+ 4h\{f\}] + 2h[2h + 6h\{2\} + 6h\{3\} \\ &+ \cdots + 6h\{f - 2\} + 4h\{f - 1\}] \\ &+ 2h[6h + 6h\{2\} + 6h\{3\} + \dots \\ &+ 6h\{f - 3\} + 4h\{f - 2\}] \\ &+ 6h[6h + 6h\{2\} + 6h\{3\} + \dots \\ &+ 6h\{f - 4\} + 4h\{f - 3\}] \\ &+ 6h[6h + 6h\{2\} + 6h\{3\} + \dots \\ &+ 6h\{f - 5\} + 4h\{f - 4\}] + \dots \\ &+ 6h[6h + 4h\{2\}] + 6h[4h]. \end{aligned}$$

After simplification, we obtain:

$$N(G[h, f]) = h^2[6f^3 + 122f - 216]. \tag{2.4}$$

Case 4: $h < 2f - 2$ and f is even.
In this case, for $G[h, f]$ we have

$$\zeta(G[h, f]) \quad = \quad \{e_1^{2h}, e_2^{4h}, e_3^{4h}, e_4^{2h}, e_5^{2h}, \dots, e_{2f-2}^{4h}, e_{2f-1}^{4h}, e_{2f}^{2h}\}.$$

Using formula (1.2), the NSC number of $G[h, f]$ is given by

$$\begin{aligned} N(G[h, f]) \quad = \quad & 4h^2\Bigg(\Bigg[\frac{(2f - 1)(2f)}{2} + (1 + 2 + 5 + 6 \\ & + \cdots + (2f - 3) + (2f - 2))\Bigg] \\ & +2\Bigg[\frac{(2f - 2)(2f - 1)}{2} + (1 + 4 + 5 + \\ & \cdots + (2f - 4) + (2f - 3))\Bigg] \\ & +2\Bigg[\frac{(2f - 3)(2f - 2)}{2} + (3 + 4 + 7 + \\ & 8 + \cdots + (2f - 5) + (2f - 4))\Bigg] \\ & +\Bigg[\frac{(2f - 4)(2f - 3)}{2} + (2 + 3 + 6 + \end{aligned}$$

$$7+\cdots+(2f-6)+(2f-5))\Big]$$
$$+\Big[\frac{(2f-5)(2f-4)}{2}+(1+2+5+6$$
$$+\cdots+(2f-7)+(2f-6))\Big]$$
$$+\cdots+\Big[\frac{3(3+1)}{2}+(1+2)\Big]+$$
$$2\Big[\frac{2(2+1)}{2}+(1)\Big]+2\Big[\frac{1(1+1)}{2}\Big]\Big).$$

After simplification we get

$$N(G[h,f])=4h^2\Big[2f^3+\frac{f}{2}(2f^2-5)\Big]. \tag{2.5}$$

Case 5: $h<2f-2$ and f is odd.
In this case, the eccentricity sequence of $G[h,f]$ is given by

$$\zeta(G[h,f]) \quad = \quad \{e_1^{2h},e_2^{4h},e_3^{4h},e_4^{2h},e_5^{2h},\ldots,e_{2f-2}^{2h},e_{2f-1}^{2h},e_{2f}^{4h}\}.$$

By formula (1.2), the NSC number of $G[h,f]$ is given by

$$\begin{aligned}N(G[h,f])=\;&2h[4h+4h\{2\}+2h\{3\}+2h\{4\}\\&+4h\{5\}+4h\{6\}+\cdots+2h\{2f-3\}\\&+2h\{2f-2\}+4h\{2f-1\}]+4h\\&[4h+2h\{2\}+2h\{3\}+4h\{4\}+4h\{5\}\\&+\cdots+2h\{2f-4\}+2h\{2f-3\}\\&+4h\{2f-2\}]+4h[2h+2h\{2\}\\&+4h\{3\}+4h\{4\}+\cdots+2h\{2f-5\}\\&+2h\{2f-4\}+4h\{2f-3\}]+2h[2h\\&+4h\{2\}+4h\{3\}+\cdots+2h\{2f-6\}\\&+2h\{2f-5\}+4h\{2f-4\}]+\ldots\\&+2h[2h+4h\{2\}+4h\{3\}+2h\{4\}\\&+2h\{5\}+4h\{6\}]+2h[4h\\&+4h\{2\}+2h\{3\}+2h\{4\}+4h\{5\}]+4h\\&[4h+2h\{2\}+2h\{3\}+4h\{4\}]+4h\\&[2h+2h\{2\}+4h\{3\}]+2h[2h\\&+4h\{2\}]+2h[4h].\end{aligned}$$

Simplifying above, we obtain

$$N(G[h,f])=4h^2[3f^3-f]. \tag{2.6}$$

This completes the proof. □

Remark. For V-phenylenic nanotori, the graph become self-centered. Therefore non-self-centrality number of V-phenylenic nanotori is zero.

3. TUC_4C_8 nanotubes

In this section, we compute the non-self centrality number of TUC_4C_8 nanotubes. In the structure of TUC_4C_8 nanotube, every C_4 cycle is adjacent to four C_8 cycles. We will denote TUC_4C_8 nanotube by $G[u, v]$, where s is the number of octagons in a fixed row and t denotes the sum of C_4 and C_8 cycles in a fixed column (see Figure 4).

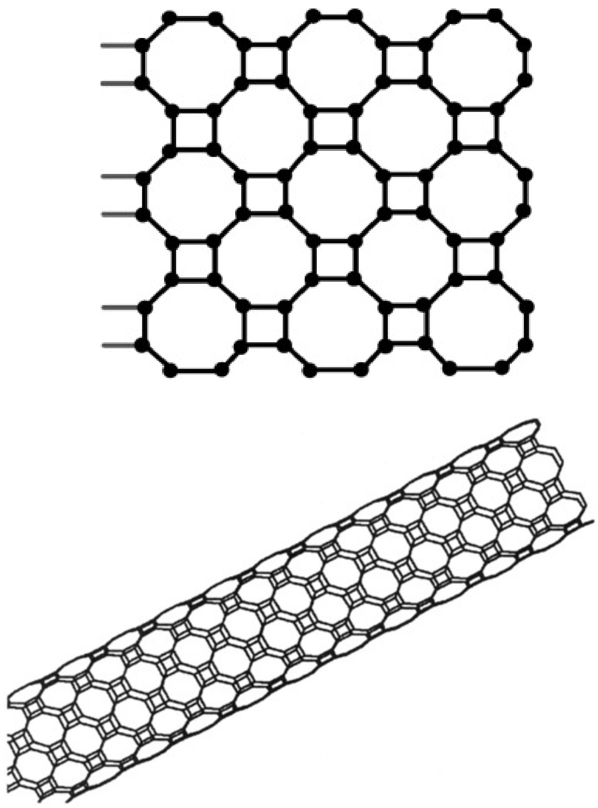

Figure 4. 2-D and 3-D structure of TUC_4C_8 Nanotube.

Consider

$$X = \{w \in \mathcal{V}(G[s, t]) \mid \deg(w) = 2\},$$

$$Y = \{w \in \mathcal{V}(G[s, t]) \mid \deg(w) = 3\}.$$

Then $|X| = 4s$ and $|Y| = 4st$. Also

$$|\mathcal{E}(G[s, t])| = 2s(3t + 2).$$

Remark. The graph $G[s, t]$ becomes self-centered for $t = 1$. Therefore the non-self-centrality number of $G[s, 1]$ is zero.

Theorem 3. Assume that $s \geq 2$ and t is an odd integer. Then the NSC number of TUC_4C_8 nanotube is given by

$$N(G[s,t]) = \frac{8s^2t}{3}(t+1)(t+2). \tag{3.1}$$

Proof. The eccentricity sequence of $G[s,t]$ is given by

$$\zeta(G[s,t]) \;=\; \{e_1^{4s}, e_2^{4s}, \ldots, e_t^{4s}, e_{t+1}^{4s}\}. \tag{3.2}$$

Using formula (1.2) the NSC of $G[s,t]$ is given by

$$\begin{aligned} N(G[s,t]) &= 16s^2[1+2+3+\cdots+(t)] + 16s^2[1+\\ &\quad 2+3+\cdots+(t-1)] + 16s^2[1+2+3\\ &\quad +\cdots+(t-2)] + \cdots + 16s^2[1+2] + 16u^2\\ &= 16s^2[1\cdot 2 + 2\cdot 3 + \cdots + (t-1)(t)\\ &\quad +(t)(t+1)]\\ &= \frac{8s^2t}{3}(t+1)(t+2). \end{aligned}$$

This completes the proof.

Remark. The graph of TUC_4C_8 nanotori, shown in Figure 5, is self-centered. Therefore non-self-centrality number of nanotori is zero.

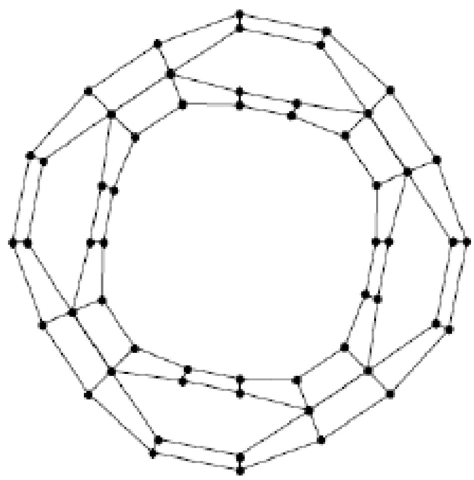

Figure 5. TUC_4C_8 nanotori.

4. Conclusions

In this paper, we computed general formulas for the non-self-centrality number of V-Phenylenic and $TUC_4C_8(R)$ nanotubes. For future study, we can calculate the non-self-centrality number of other molecular structures such as α-Boron nanotubes, some layer structures and dendrimers.

Conflict of interest

The authors have no conflict of interest to declare.

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