

COMPUTING MODIFIED ECCENTRIC CONNECTIVITY INDEX AND CONNECTIVE ECCENTRIC INDEX OF V-PHENYLENIC NANOTORUS

NILANJAN DE^{a,*}, SK. MD. ABU NAYEEM^b and ANITA PAL^c

ABSTRACT. The modified eccentric connectivity index of a molecular graph is defined as the sum, of the products of eccentricity with the total degree of neighbouring vertices, over all vertices of the graph. On the other hand, the connective eccentric index of a graph is defined as the sum of the ratio of degree and eccentricity of the vertices. In this paper the exact expressions for the modified eccentric connectivity index and connective eccentric index of V-phenylenic nanotorus are computed.

Keywords: *Eccentricity, V-phenylenic nanotorus, modified eccentric connectivity index, connective eccentric index.*

INTRODUCTION

Topological indices are numeric quantities of a molecular graph G , which are invariants under the symmetry properties of G . In recent years a number of graph invariants related to vertex eccentricity have been derived and studied. Let G be a simple connected molecular graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, let $\deg(v)$ denotes the number of first neighbor of v . The distance between the vertices u and v of G is equal to the length, that is the number of edges, of the shortest path connecting u and v and we denote it by $d(u, v)$. For a given vertex v , its eccentricity $\varepsilon(v)$ is the largest distance from v to any other vertices of G . If $N(v) = \{u \in V(G) : uv = e \in E(G)\}$, then the modified eccentric connectivity index of any graph is defined as

$$\xi_c(G) = \sum_{v \in V(G)} \delta(v) \varepsilon(v) \quad (1)$$

^a Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India.

^b Department of Mathematics, Aliah University, Kolkata, India.

^c Department of Mathematics, National Institute of Technology, Durgapur, India.

* Corresponding author: de.nilanjan@rediffmail.com

where, $\delta(v) = \sum_{u \in N(v)} \deg(u)$. There are several chemical as well as mathematical studies of this modified eccentric connectivity index and polynomial. In [1], the modified eccentric connectivity polynomial for three infinite classes of fullerenes was computed. In [2], a numerical method for computing modified eccentric connectivity polynomial and modified eccentric connectivity index of one-pentagonal carbon nanocones was presented. In [3], some exact formulas for the modified eccentric connectivity polynomial of Cartesian product, symmetric difference, disjunction and join of graphs were presented. Some upper and lower bounds for this modified eccentric connectivity index was recently studied by the present authors in [4]. Also in [5] modified eccentric connectivity index of generalized thorn graphs was presented.

Another vertex eccentricity based topological index, named the connective eccentricity index, was introduced by Gupta, Singh and Madan [6] and is defined as

$$C^e(G) = \sum_{v \in V(G)} \deg(v) \varepsilon(v)^{-1} \quad (2)$$

In [7], M. Ghorbani gave some bounds of connective eccentricity index and also computed this index for two infinite classes of dendrimers. The eccentric connectivity index and the connective eccentric index of an infinite family of fullerenes was computed in [9] by Ghorbani and Malekjani. Yu and Feng, in [10] derived some upper or lower bounds for the connective eccentric index and investigated the maximal and the minimal values of connective eccentricity index among all n -vertex graphs with fixed number of pendent vertices. De [8] reported some bounds for this index in terms of some graph invariants. In [11] different graph operations of connective eccentric index were reported.

Carbon nanotubes are rolled-up sheets of graphite and if its ends meet, a nanotorus is produced. In this paper, we consider V -phenylenic nanotorus where the phenylenic lattice can be constructed from a square net embedded on the toroidal surface [17]. In figure 1, the molecular graph of V -phenylenic nanotorus is constructed from 4-, 6-, 8- gons. Studies of different topological indices of this nanotorus were reported in [12-16]. Let, in the two-dimensional lattice of V -phenylenic nanotorus, p denotes the number of hexagons in a fixed row and q denotes the number of hexagons in a fixed column, so that V -phenylenic nanotorus (TO) can be represented as $TO(p,q)$. The molecular graph of this nanotorus $TO(4,5)$ is given in Figure 1. For V -phenylenic nanotorus it is clear that, $|V(TO)| = 6pq$ and $|E(TO)| = 9pq$. Let u, v be two different vertices of TO. Then, we notice that $\varepsilon(u) = \varepsilon(v)$ and V -phenylenic nanotorus is cubic and thus for all $v \in V(TO)$, $\deg(v) = 3$. In this paper we derive some exact expressions for the modified eccentric connectivity index and the connective eccentric index of V -phenylenic nanotorus is computed.

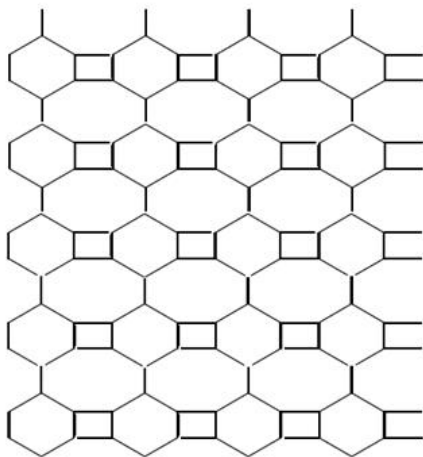


Figure 1. V-Phenylenic Nanotorus, $TO[4,5]$.

MAIN RESULTS

The main aim of this section is to compute the modified eccentric connectivity index and connective eccentric index of the molecular graph of a V-phenylenic nanotorus for different values of p and q . Let us first consider the modified eccentric connectivity index of V-phenylenic nanotorus.

Proposition 1

Let p and q be even integers. Then the modified eccentric connectivity index of V-phenylenic nanotorus is computed as follows

$$\xi_c(TO) = \begin{cases} 27pq(p+4q) & \text{if } q \geq p \\ 27pq(3p+2q) & \text{if } q \leq p \end{cases}$$

Proof: Since, a V-phenylenic nanotorus is cubic, so for all $v \in V(TO)$, $\delta(v) = 9$. We first assume that $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p}{2} = \frac{1}{2}(4q + p).$$

Thus, from (1)

$$\xi_c(TO) = \sum_{v \in V(TO)} \delta(v) \varepsilon(v) = \sum_{v \in V(TO)} \frac{9}{2} (4q + p) = \frac{9}{2} (p + 4q) \times |V(TO)|.$$

Again, if $q \leq p$ then for all $v \in V(TO)$, $\varepsilon(v) = q + \frac{3p}{2} = \frac{1}{2}(3p + 2q)$.

Hence, from (1)

$$\xi_c(TO) = \sum_{v \in V(TO)} \delta(v) \varepsilon(v) = \sum_{v \in V(TO)} \frac{9}{2} (3p + 2q) = \frac{9}{2} (3p + 4q) \times |V(TO)|.$$

which completes the proof. \square

Proposition 2

Let p and q be odd integers. Then the modified eccentric connectivity index of V-phenylenic nanotorus is computed as follows

$$\xi_c(TO) = \begin{cases} 27pq(p + 4q - 1) & \text{if } q \geq p \\ 27pq(3p + 2q - 1) & \text{if } q \leq p. \end{cases}$$

Proof: Suppose, $q \geq p$, then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p-1}{2} = \frac{1}{2}(4q + p - 1).$$

Also if $q \leq p$ then for all $v \in V(TO)$,

$$\varepsilon(v) = q + \frac{3p-1}{2} = \frac{1}{2}(3p + 2q - 1).$$

Since, for a V-phenylenic nanotorus $\delta(v) = 9$, for all $v \in V(TO)$, therefore the desired result follows similarly.

Proposition 3

Let p be even and q be odd integers. Then the modified eccentric connectivity index of V-phenylenic nanotorus is computed as follows

$$\xi_c(TO) = \begin{cases} 27pq(p + 4q) & \text{if } q \geq p \\ 27pq(3p + 2q) & \text{if } q \leq p. \end{cases}$$

Proof: Let us assume that $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p}{2} = \frac{1}{2}(4q + p).$$

Thus, from (1)

$$\xi_c(TO) = \sum_{v \in V(TO)} \delta(v) \varepsilon(v) = \sum_{v \in V(TO)} \frac{9}{2} (4q + p) = \frac{9}{2} (p + 4q) \times |V(TO)|.$$

Again, if $q \leq p$ then for all $v \in V(TO)$, $\varepsilon(v) = q + \frac{3p}{2} = \frac{1}{2}(3p + 2q)$.

Therefore, from (1) we get

$$\xi_c(TO) = \sum_{v \in V(TO)} \delta(v) \varepsilon(v) = \sum_{v \in V(TO)} \frac{9}{2}(3p + 2q) = \frac{9}{2}(3p + 4q) \times |V(TO)|$$

from where the desired result follows. \square

Proposition 4

Let p be odd and q be even integers. Then the modified eccentric connectivity index of V-phenylenic nanotorus is computed as follows

$$\xi_c(TO) = \begin{cases} 27pq(p + 4q - 1) & \text{if } q \geq p \\ 27pq(3p + 2q - 1) & \text{if } q \leq p. \end{cases}$$

Proof: Let, $q \geq p$, then all the vertices of TO are of eccentricity $2q + \frac{p-1}{2} = \frac{1}{2}(4q + p - 1)$.

Similarly, if $q \leq p$, then the eccentricity of all the vertices of TO is equal to $q + \frac{3p-1}{2} = \frac{1}{2}(3p + 2q - 1)$.

Since, for a V-phenylenic nanotorus all the vertices are of degree 3, therefore the desired result follows similarly. \square

The above results can be summarized as follows:

Theorem 1

Let p be even, then the modified eccentric connectivity index of V-phenylenic nanotorus is given by

$$\xi_c(TO) = \begin{cases} 27pq(p + 4q) & \text{if } q \geq p \\ 27pq(3p + 2q) & \text{if } q \leq p \end{cases}$$

and if p be odd, then the modified eccentric connectivity index of V-phenylenic nanotorus is given by

$$\xi_c(TO) = \begin{cases} 27pq(p + 4q - 1) & \text{if } q \geq p \\ 27pq(3p + 2q - 1) & \text{if } q \leq p. \end{cases}$$

Now we compute connective eccentric index of the molecular graph of a V-phenylenic nanotorus for different values of p and q .

Proposition 5

Let p and q be even integers. Then the connective eccentric index of V -phenylenic nanotorus is computed as follows

$$C^{\varepsilon}(TO) = \begin{cases} \frac{36pq}{(p+4q)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q)} & \text{if } q \leq p. \end{cases}$$

Proof: First, assume that $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p}{2} = \frac{1}{2}(4q + p).$$

Therefore, from (2) we have

$$C^{\varepsilon}(TO) = \sum_{v \in V(TO)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(TO)} \frac{6}{(p+4q)} = |V(TO)| \times \frac{6}{(p+4q)}.$$

Again if $q \leq p$ then for all $v \in V(TO)$, $\varepsilon(v) = q + \frac{3p}{2} = \frac{1}{2}(3p + 2q)$.

Thus, using (2) we have

$$C^{\varepsilon}(TO) = \sum_{v \in V(TO)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(TO)} \frac{6}{(3p+2q)} = |V(TO)| \times \frac{6}{(3p+2q)}$$

which completes the proof. \square

Proposition 6

Let p and q be odd integers. Then the connective eccentric index of V -phenylenic nanotorus is computed as follows

$$C^{\varepsilon}(TO) = \begin{cases} \frac{36pq}{(p+4q-1)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q-1)} & \text{if } q \leq p. \end{cases}$$

Proof: Let, $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p-1}{2} = \frac{1}{2}(4q + p - 1).$$

Again if $q \leq p$ then for all $v \in V(TO)$,

$$\varepsilon(v) = q + \frac{3p-1}{2} = \frac{1}{2}(3p+2q-1).$$

Since, for a V-phenylenic nanotorus all the vertices are of degree 3, therefore applying a similar argument as Proposition 5, we get the result. \square

Proposition 7

Let p be even and q be odd integers. Then the connective eccentric index of V-phenylenic nanotorus is computed as follows

$$C^\varepsilon(TO) = \begin{cases} \frac{36pq}{(p+4q)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q)} & \text{if } q \leq p. \end{cases}$$

Proof: We first assume that $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p}{2} = \frac{1}{2}(4q+p).$$

$$\text{Thus, from (2) } C^\varepsilon(TO) = \sum_{v \in V(TO)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(TO)} \frac{6}{(p+4q)} = |V(TO)| \times \frac{6}{(p+4q)}.$$

$$\text{Again if, } q \leq p \text{ then for all } v \in V(TO), \varepsilon(v) = q + \frac{3p}{2} = \frac{1}{2}(3p+2q).$$

Therefore, from (2),

$$C^\varepsilon(TO) = \sum_{v \in V(TO)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(TO)} \frac{6}{(3p+2q)} = |V(TO)| \times \frac{6}{(3p+2q)},$$

which completes the proof. \square

Proposition 8

Let p be odd and q be even integers. Then the connective eccentric index of V-phenylenic nanotorus is computed as follows

$$C^\varepsilon(TO) = \begin{cases} \frac{36pq}{(p+4q-1)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q-1)} & \text{if } q \leq p. \end{cases}$$

Proof: Let us first assume that, $q \geq p$. Then for all $v \in V(TO)$,

$$\varepsilon(v) = 2q + \frac{p-1}{2} = \frac{1}{2}(4q + p - 1).$$

Again if $q \leq p$ then for all $v \in V(TO)$, $\varepsilon(v) = q + \frac{3p-1}{2} = \frac{1}{2}(3p + 2q - 1).$

Since, for a V-phenylenic nanotorus all the vertices are of degree 3, therefore following a similar argument as Proposition 7, we get the result. \square

The propositions 5, 6, 7 and 8 can be summarized as follows:

Theorem 2

Let p be even, then the connective eccentric index of V-phenylenic nanotorus is given by

$$C^{\varepsilon}(TO) = \begin{cases} \frac{36pq}{(p+4q)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q)} & \text{if } q \leq p. \end{cases}$$

and if p be odd, then the connective eccentric index of V-phenylenic nanotorus is given by

$$C^{\varepsilon}(TO) = \begin{cases} \frac{36pq}{(p+4q-1)} & \text{if } q \geq p \\ \frac{36pq}{(3p+2q-1)} & \text{if } q \leq p. \end{cases}$$

CONCLUSIONS

In this paper, we studied the V-phenylenic nanotorus. As our main result, we have derived exact formulas for the modified eccentric connectivity index and connective eccentric index of V-phenylenic nanotorus. For further study, lower and an upper bound for these topological indices of V-phenylenic nanotorus can be computed.

REFERENCES

1. A.R. Ashrafi, M. Ghorbani, *Electronic Materials Letters*, **2010**, 6(2), 87.
2. M. Alaeiyan, J. Asadpour, R. Mojarad, *Fullerenes, Nanotubes and Carbon Nanostructures*, **2013**, 21(10), 825.
3. A.R. Ashrafi, M. Ghorbani, M.A. Hossein-Zadeh, *Serdica Journal of Computing*, **2011**, 5, 101.
4. N. De, S.M.A. Nayeem, A. Pal, *Advanced Modeling and Optimization*, **2014**, 16(1), 133.

5. N. De, A. Pal, S.M.A. Nayeem, Modified eccentric connectivity of generalized thorn graphs, *International Journal of Computational Mathematics* (To appear).
6. S. Gupta, M. Singh, A.K. Madan, *Journal of Molecular Graphics and Modelling*, **2000**, 18, 18.
7. M. Ghorbani, *Journal of Mathematical Nanoscience*, **2011**, 1, 43.
8. N. De, *International Journal of Contemporary Mathematical Sciences*, **2012**, 7(44), 2161.
9. M. Ghorbani, K. Malekjani, *Serdica Journal of Computing*, **2012**, 6, 299.
10. G. Yu, L. Feng, *MATCH communications in mathematical and in computer chemistry*, **2013**, 69, 611.
11. N. De, A. Pal, S.M.A. Nayeem, On some bounds and exact formulae for connective eccentric indices of graphs under some graph operations, *International Journal of Combinatorics* (To appear).
12. A.R. Ashrafi, M. Ghorbani, M. Jalali, *Indian Journal of Chemistry*, **2008**, 47A, 535.
13. H. Yousefi-Azari, J. Yazdani, A. Bahrami, A.R. Ashrafi, *Journal of Serbian Chemical Society*, **2007**, 72(11) 1063.
14. V. Alamian, A. Bahrami, B. Edalatzaheh, *International Journal of Molecular Sciences*, **2008**, 9(3), 229.
15. M. Ghorbani, H. Mesgarani, S. Shakeraneh, *Optoelectronics and advanced materials*, **2011**, 5(3), 324.
16. Z. Yarahmadi, A.R. Ashrafi, S. Moradi, *Journal of Applied Mathematics and Computing*, **2014**, 45(1-2), 35.
17. M.V. Diudea, *Fullerenes, Nanotubes and Carbon Nanostructures*, **2002**, 10, 273.