OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 9, No. 9-10, September – October 2015, p.1221-1223

# Computing the edge Szeged index of polyhex nanotori by automorphism

JAFAR ASADPOUR[a*], RASOUL MOJARAD[b], MEHDI ALAEIYAN[C]
[a]*Department of Mathematics, Miyaneh Branch, Islamic Azad University, Miyaneh, Iran*
[b]*Department of Science , Boushehr Branch, Islamic Azad University, Boushehr, Iran*
[c]*Department of Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran*

Let *G* be a molecular graph and *e*=*uv* be an edge of *G*. Define $n_{eu}(e\,|\,G)$ to the number of edges of lying closer to *u* than to *v* and $n_{ev}(e\,|\,G)$ to the number of edges of lying closer to *v* than to *u*. Then the edge Szeged index of *G*, $Sz_e(G)$, is defined as the sum of $n_{eu}(e\,|\,G)\,n_{ev}(e\,|\,G)$ over all edges of *G*. In this paper we find the above index for $TUC_4C_8(S)$ nanotori graph using the group of automorphisms of *G*. This is an efficient method of finding this index especially when the automorphism group of *G* has a few orbits on *E*(*G*).

(Received October 30, 2014; accepted 9, 2015)

*Keywords:* Edge Szeged Index, Nanotori, automorphism

## 1. Introduction

A graph *G* consists of a set of vertices *V*(*G*) and a set of edges *E*(*G*). The vertices in *G* are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices *u* and *v* in *G* such that $u, v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively.

Topological indices are graph invariants and are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies [9,11]. Many topological indices have been defined and several of them have found applications as means to model physical, chemical, pharmaceutical and other properties of molecules [13]. The oldest topological index is the Wiener index which was introduced by Harold wiener [15]. Here, we consider a new topological index, named edge Szeged index, see [14].

To define the edge Szeged index of a connected graph *G*, we correspond to an edge *e*=*uv* of *E*(*G*), two quantities $n_{eu}(e\,|\,G)$ and $n_{ev}(e\,|\,G)$ in which $n_{eu}(e\,|\,G)$ is the number of edges lying closer to the vertex *u* than the vertex *v*, and $n_{ev}(e\,|\,G)$ is the number of edges lying closer to the vertex *v* than the vertex *u*. Then the edge Szeged index of the graph *G* is defined as

$$Sz_e(G) = \sum_{e=uv\in E} n_{eu}(e\,|\,G)\,n_{ev}(e\,|\,G)$$

Let *e*=*uv* be an edge of *G*. We define the following sets:

$$N_u(e\,|\,G) = \{w \in V(G)\,|\,d(u,w) < d(v,w)\},$$
$$N_v(e\,|\,G) = \{w \in V(G)\,|\,d(v,w) < d(u,w)\},$$

$N_0(e\,|\,G) = \{w \in V(G)\,|\,d(v,w) = d(u,w)\}$. If the size of $N_0(e\,|\,G)$ is zero, then $n_{eu}(e\,|\,G)$ (resp. $n_{ev}(e\,|\,G)$) is the number of edges of in graph introduce by $N_u(e\,|\,G)$ (resp. $N_v(e\,|\,G)$).

We using the above notation that compute the edge Szeged index.

By an automorphism of the graph *G* =(*V*,*E*) we mean a bijection $\sigma$ on *V* which preserves the edge set *E*, i.e., if *e*=*uv* is an edge, then $e^{\sigma} = u^{\sigma}v^{\sigma}$ is an edge of *E*. Here $u^{\sigma}$ denotes the image of the vertex *u* under $\sigma$ . It is obvious that the set of all the automorphisms of *G* under the composition of mappings forms a group which is denoted by $\Gamma = Aut(G)$. We say that Γ acts transitively on *E*(*G*) if for any edges *e* and *f* in *E* there is $\sigma \in \Gamma$ such that $e^{\sigma} = f$ .

The following result enables us to calculate $Sz_e(G)$ easily.

**Lemma 1.** Let *G* = *(V , E)* be a simple connected graph. If Aut*(G)* on *E* has orbits $E_1, E_2, \ldots, E_r$ with representatives $e_1, e_2, \ldots, e_r$, respectively, where $e_i = u_i v_i$, then $Sz_e(G) = \sum_{i=1}^{r} |E_i|\, n_{e_i u_i}(e_i\,|\,G)\, n_{e_i v_i}(e_i\,|\,G)$.

**Proof.** Since each orbit $E_i$ acting transitively on $E_i$, so $n_{e_i u_i}(e_i\,|\,G)$ and $n_{e_i v_i}(e_i\,|\,G)$ are constant for all edges $e_i = u_i v_i$ in orbit $E_i$. Now by definition edge Szeged index we have

$$Sz_e(G) = \sum_{e=uv} n_{eu}(e|G)n_{ev}(e|G) =$$

$$\sum_{i=1}^{r} \sum_{e_i=u_iv_i} n_{e_iu_i}(e_i|G)n_{e_iv_i}(e_i|G) =$$

$$\sum_{i=1}^{r} |E_i| n_{e_iu_i}(e_i|G)n_{e_iv_i}(e_i|G)$$

The proof is completed.

Some topological indices are computed for some nanotubes and nanotori, for example see [1,2,4,5,6,12,16]. In this paper we compute the edge Szeged index of $TUC_4C_8(S)$ nanotori, using the group of automorphisms of *G*.

## 2. Main results and discussion

We assume that $T = TUC_4C_8(S)[m,n]$ is the molecular graph of a $TUC_4C_8(S)$ nanotorus with *m* and *n* oblique edges in each row and column (Fig. 1). This graph has 2*n* rows with *m* vertices in each row and 2*m* columns with *n* vertices in each column. Hence graph *T* has exactly 2*mn* vertices and 3*mn* edges.

The following lemma is basic.

**Lemma 2 ([3]).** The automorphism group *T* on the set of edges has exactly three orbits determined by a vertical edge, a horizontal edge and an oblique edge of T.

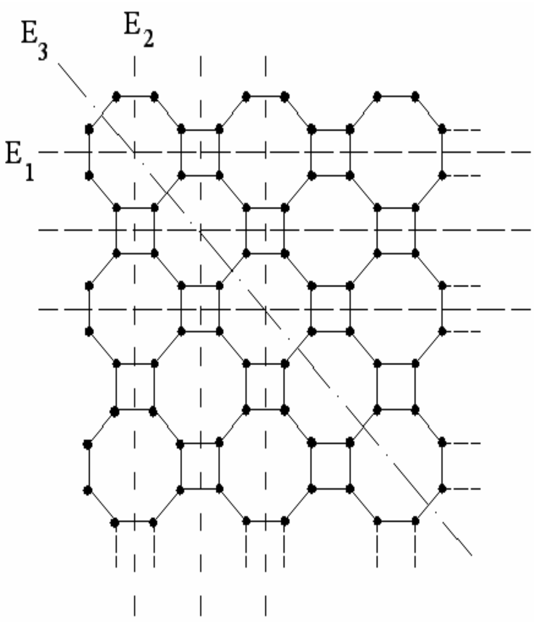


*Fig. 1. The 2-Dimensional Lattice of* $T = TUC_4C_8(S)[3,3]$ *Nanotorus*

Now we ready to compute the edge Szeged index of $TUC_4C_8(S)$.

**Theorem 1**. The edge Szeged of nanotori $T = TUC_4C_8(S)[m,n]$ is

$$Sz_e(T) = \frac{mn}{4} \times \begin{cases} 27n^2m^2 - 30n^2m - 12nm^2 + \\ 12nm + 13n^2 + 4m^2 - 12n + 4 & n \le m \\ \\ 27n^2m^2 - 30nm^2 - 12n^2m + \\ 12nm + 13m^2 + 4n^2 - 12m + 4 & n > m \end{cases}$$

**Proof.** Let the orbits of *Aut*(*T*) on the set of edges of *T* be denoted by $E_1$ (horizontal edges), $E_2$ (vertical edges) and $E_3$ (oblique edges), according Lemma 2 (Fig. 2). So by Lemma 1, we have

$$Sz_e(T) = \sum_{i=1}^{3} |E_i| n_{e_iu_i}(e_i|T)n_{e_iv_i}(e_i|T).$$

Consider the edge *e*=*uv* in the orbit $E_i$ for $i = 1,2,3$. Now we count $n_{eu}(e|T)$ which is the number of edges of the set $N_u(e|T)$.

Case 1. Suppose *e*=*uv* be the horizontal edge in orbit $E_1$. Let us choose $u = u_{2m}$ and $v = u_{2(m+1)}$ as vertices of the edge *e*=*uv* (Fig. 3). The set $N_u(e|T)$ consist vertices of columns $C_1, C_2, \ldots, C_m$. Since each column has *n* vertices, so the size of $N_u(e|T)$ is *mn*. It is easy to check that the vertices of columns $C_1$ and $C_m$ have degree 2 and other vertices are from degree 3. Therefore $n_{eu}(e|T) = \frac{1}{2}(3mn - 2n)$. In a similar manner we obtain $n_{ev}(e|T) = \frac{1}{2}(3mn - 2n)$.

Case 2. Let *e*=*uv* be the vertical edge in orbit $E_2$. Suppose $T' = T'[m',n']$ is a rotation of *T* through $\frac{\pi}{2}$, where $m' = n$ and $n' = m$. Apply case 1, we have $n_{eu}(e|T) = n_{ev}(e|T) = \frac{1}{2}(3mn - 2m)$.

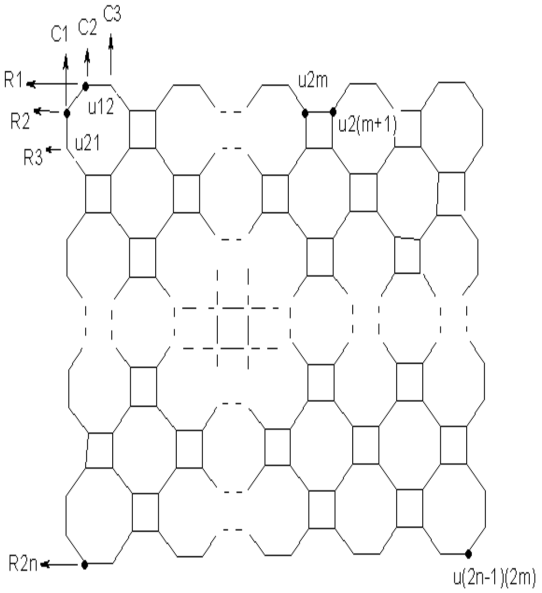


*Fig. 2. The vertices, rows and columns.*

Case 3. Let $e=uv$ be the oblique edge in orbit $E_3$. Let us choose $u=u_{21}$ and $v=u_{12}$ as vertices of the edge $e=uv$, (Fig. 2). We first assume $n \ge m$. The set $N_u(e|T)$ consist vertices of rows $R_4, R_5, \ldots, R_{n+1}$ and the half vertices of rows $R_1, R_2, R_3, R_n$. Since each row has $m$ vertices. Hence

$|N_u(e|T)| = m(n-2) + 4(\frac{m}{2}) = mn$. The number of vertices of the set $N_u(e|T)$ that its degree is 2 equal to $3m$-2 and other vertices have degree 3. Therefore $n_{eu}(e|T) = \frac{1}{2}(3mn - 3n + 2)$. Since $T$ is symmetric, so

$$n_{ev}(e|T) = \frac{1}{2}(3mn - 3n + 2).$$

Now if $n<m$, then in a similar manner we obtain

$$n_{eu}(e|T) = n_{ev}(e|T) = \frac{1}{2}(3mn - 3m + 2).$$

Since $|E_i| = mn$ for $i = 1,2,3$, so with an easy calculations the proof complete.

## References

[1] S. Alikhani, M. A. Iranmanesh, Digest Journal of Nanomaterials and Biostructures , **5**(1), 1 ( 2010).
[2] J. Asadpour, R. Mojarad, L. Safikhani, Digest Journal of Nanomaterials and Biostructures, **6**( 3), 937 (2011).
[3] A. Ashrafi, Sh. Yousefi, Digest Journal of Nanomaterials and Biostructures, **4**, 407 (2009).
[4] A. R. Ashrafi, Sh. Yousefi, Nanoscale MATCH Commun. Math. Comput. Chem., **57,** 403 (2007).
[5] J. Asadpour, Proc. Rom. Acad., Series B, 15(3), 157 (2013).
[6] J. Asadpour, Digest Journal of Nanomaterials and Biostructures, **7**( 1), 19 (2012).
[7] J. Asadpour, Optelectron. Adv. Mater–Rapid Comm., **5,** 937 (2011).
[8] J. Asadpour, R. Mojarad, B. Daneshian, Studia ubb chemia, **4**, 157 (2014).
[9] A. T. Balaban (Eds). “Topological Indices and Related Descriptors in QSAR and QSPR”, Gordon and Breach Science Publishers, The Netherlands, (1999).
[10] B. Daneshian, A. Nemati, R. Mojarad, J. Asadpour, Optelectronics Adv. Mater–Rapid Comm., **8,** 985 (2014).
[11] I. Gutman, O. E. Polansky. “Mathematical Concepts in Organic Chemistry”, Springer- Verlag, New York, (1986).
[12] A. Heydari, B. Taeri, European Journal of Combinatorics, **30**, 1134 (2009)
[13] M. A. Johnson, G. M. Maggiora, “Concepts and Applications of Molecular Similarity”, Wiley Interscience, New York (1990).
[14] I. Gutman, A. R. Ashrafi, Croat. Chem. Acta. **81**(2), 263 (2008).
[15] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[16] H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalifeh, Digest Journal of Nanomaterials and Biostructures, **3**(4), 251 (2008).

*Corresponding author: jafar_asadpour@yahoo.com