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Computing Wiener and Szeged Indices of an Achiral Polyhex Nanotorus

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Abstract

Suppose G is the molecular graph of an achiral polyhex nanotorus and e is an edge of G. We denote by $N_1(e|G)$ the number of vertices of G lying closer to one end of e and by $N_2(e|G)$ the number of vertices of G lying closer to the other end of e. Then the Szeged index of G is defined as $Sz(G) = \sum_{e\in E(G)} N_1(e|G)N_2(e|G)$, where E(G) is the set of all edges of G. The Wiener index of G is defined as $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)} d(x,y)$, where d(x,y) denotes the length of a minimal path between x and y. In this paper, the Wiener and Szeged indices of an achiral polyhex nanotorus are computed.

Keywords: Achiral polyhex nanotorus, Wiener index, Szeged index.

Introduction

Graph representation of molecular structures is widely used in computational and theoretical chemistry (Trinajstic 1992, Bonchev 1983, Rouvray 1983, Balaban 1985). Trinajstic (1992) noted that the roots of chemical graph theory may be found in the works by chemists of 18-19th centuries such as Higgins, Kopp and Crum Brown. First chemical graphs for representing molecules were used by them. Recently, Konstantinova and Skorobogatov (2001) showed that chemical hypergraph is also useful in investigating structure–properties relationship (QSPR).

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.

To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices could be used too. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made by the chemist (Harold Wiener 1947). In that year, he introduced the notion of path number of a graph as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds.

Hosoya (1971) reformulated the Wiener index in terms of distances between vertices in an arbitrary graph. He defined W as the sum of distances between all pairs of vertices of the graph under consideration, $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)} d(x,y)$, where d(u,v) is the number of edges in a minimum path connecting the vertices u and v. We encourage the reader to consult the special issues of MATCH Communication in Mathematics and in Computer Chemistry (Gutman *et al.,* 1997a) and Discrete Applied Mathematics (Gutman *et al.,* 1997b) and (Diudea & Gutman 1998, Dobrynin *et al.,* 2001; Dobrynin *et al.,* 2002) for information on results on the Wiener index, the chemical meaning of the index and its history.

In the 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to W. Szeged index is one of these topological indices, which is introduced by Ivan Gutman (1994).

We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops. If e is an edge of G, connecting the vertices u and v then we write e = uv. Let

$N_1(e|G)$ be the number of vertices of G lying closer to one end of e and $N_2(e|G)$ be the number of vertices of G lying closer to the other end of e. Edges equidistance from both the ends of an edge are not taken into account. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e\in E(G)} N_1(e|G)N_2(e|G)$.

Throughout this paper our notation is standard and taken from the book of Trinajestic[1]. Our notation related nanotorus is taken from the papers by Diudea and his co-authors (John & Diudea 2004, Diudea *et al.,* 2004, Diudea *et al.,* 2003; Diudea 2002a, Diudea 2002b, Diudea & Kirby 2001). We encourage the reader to consult these papers for background material on this topic, as well as basic computational techniques. Some of the present authors (Yousefi & Ashrafi 2006, Yousefi & Ashrafi 2007, Ashrafi & Yousefi 2007a, Ashrafi & Yousefi 2007b) computed the Wiener index of polyhex, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotori. The goal of this paper is to present a new method for such calculations. As a particular case of our method, the Szeged index of an achiral polyhex nanotorus is computed for the first time.

Results and Discussion

In this section, the Wiener and Szeged indices of an achiral polyhex nanotorus is computed. We first investigate the Wiener index of these nanotori. Let us recall some definitions and notations. An automorphism of a graph G is a permutation g of the vertex set V(G) of G with the property that, for any vertices u and v, g(u) and g(v) are adjacent if and only if u is adjacent to v. The set of all automorphisms of a graph G, with the operation of the composition of permutations, is a permutation group on V(G), denoted Aut(G).

In mathematics, groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group acts like a bijective map on some set. To clarify this notion, we assume that G is a group and X is a set. G is said to act on X when there is a map $\varphi : G \times X \rightarrow X$ such that all elements $x\in X$ (i) $\varphi(e,x) = x$, where e is the identity element of G, and,(ii) $\varphi(g,\varphi(h,x)) = \varphi(gh,x)$ for all $g, h\in G$. In this case, G is called a transformation group, X is called a G-set, and φ is called the group action. For simplicity we define $gx = \varphi(g,x)$. In a group action, a group permutes the elements of X .The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given X ,the set $\{gx \mid g \in G\}$, where the group action moves x, is called the group orbit of x. If G has exactly one orbit, then G is said to be transitive. A graph G is vertex transitive if its automorphism group acts transitively on V(G). Throughout this paper T = T[p,q] denotes a polyhex achiral nanotorus of perimeter p and length q.

To compute the Wiener index of an achiral polyhex nanotorus, we first prove its graph is vertex transitive. This gives a new method for computing the Wiener index of an achiral polyhex nanotorus different from those given by some of the present authors (Yousefi & Ashrafi 2006).

Lemma 1. The molecular graph of an achiral polyhex nanotorus is vertex transitive.

Proof. To prove this lemma, we first notice that p and q must be even. Consider the vertices u_{ij} and u_{rs} of the molecular graph of an achiral polyhex nanotorus T = T[p,q], Figures 1 and 2. Suppose both of i and r are odd or even and σ is a horizontal symmetry plane which maps u_{it} to u_{rt}, $1 \le t \le p$ and π is a vertical symmetry which maps u_{tj} to u_{ts}, $1 \le t \le q$. Then σ and π are automorphisms of T and we have $\pi\sigma(u_{ij}) = \pi(u_{rj}) = u_{rs}$. Thus u_{ij} and u_{rs} are in the same orbit under the action of Aut(G) on V(G). On the other hand, the map θ defined by:

$$\theta(u_{ij}) = \theta(u_{(p+1-i)j})$$

is a graph automorphism of T and so if "i is odd and r is even" or "i is even and r is odd" then again u_{ij} and u_{rs} will be in the same orbit of Aut(T), proving the lemma.

Fig. 1. An Achiral Polyhex Nanotorus.

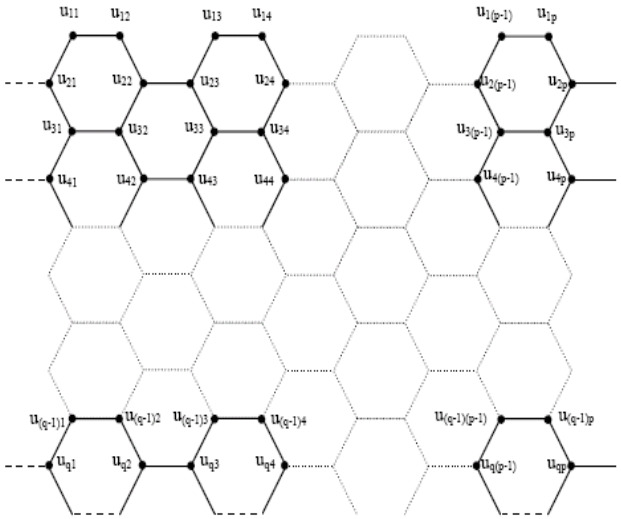

Fig. 2. A 2-Dimensional Lattice for an Achiral Polyhex Nanotorus T[p,q].

Suppose d(x) denotes the summation of topological distances between x and all vertices of G. Then we have:

Lemma 2. If G is a vertex transitive graph then for every vertices u and v, d(u) = d(v). In particular, W(G) = (n/2)d(x), where n = |V(G)| and x is a fixed vertex of G.

Proof. By assumption, there is an automorphism φ such that φ(u) = v. By definition of an automorphism, for every vertex x:

$$d(u) = \Sigma_{x\in V(G)}d(x,u) = \Sigma_{x\in V(G)}d(\varphi(x),\varphi(u))$$
$$= \Sigma_{x\in V(G)}d(\varphi(x), v) = \Sigma_{y\in V(G)}d(y,v) = d(v).$$

Therefore, $W(G) = 1/2\Sigma_{\{x,y\}\subseteq V(G)}d(x,y) = 1/2\Sigma_x d(x) = n/2d(x)$.

By Lemmas 1 and 2, in an achiral polyhex nanotorus T = T[p,q] we have W(T) = (pq/2)d(x), for a fixed vertex x of T. By this result we have:

Theorem. If T = T[p,q] is a polyhex nanotorus then the Wiener index of T is as follows:

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2+q^2-4) & q<p \\ \frac{p^2q}{24}(3q^2+3pq+p^2-4) & q\geq p \end{cases}.$$

We now compute the Szeged index of the molecular graph of an achiral polyhex nanotorus T.

Lemma 3. If e is an arbitrary edge of T = T[p,q] then $N_1(e|G) = N_2(e|G) = pq/2$. In particular, $Sz(T) = 3/8p^3q^3$.

Proof. We first assume that e is an arbitrary edge of the 2-dimensional lattice of T, Figure 2. Using symmetry of an achiral polyhex nanotorus, it is easy to see that $N_1(e|T)N_2(e|T) = N_1(f|T)N_2(f|T)$, where $f = u_{11}u_{12}$. Suppose $d(u_{ij},u_{11}) = a_{ij}$, $d(u_{ij},u_{12}) = x_{ij}$, $A = [a_{ij}]$ and $X = [x_{ij}]$. Then we have:

$$x_{i,j} = \begin{cases} a_{i,j}-1 & 2\leq j\leq \frac{n}{2}+1 \\ a_{i,j}+1 & j=1 \text{ or } j>\frac{n}{2}+1 \end{cases}.$$

Therefore for one half of pairs (i,j), we have $x_{ij} > a_{ij}$. This shows that $N_1(e|T) = N_2(e|T) = pq/2$. Next by definition of Szeged index and Lemma 2, we have:

$$Sz(T) = \sum_{e\in E(G)}N_1(e|T)N_2(e|T)$$
$$= \sum_{e\in E(G)}(pq/2)(pq/2)$$
$$= 3/2pq(1/4p^2q^2).$$

Second Proof. If G is connected bipartite graph with n vertices and m edges then by a theorem of Gutman and Dobrynin (1994),

$$Sz(G) = \frac{1}{4}\left(n^2m - \sum_{uv\in E(G)}(d(u)-d(v))^2\right).$$

Now if G = T[p,q] then by Lemma 2, d(u) = d(v) and so:

$$Sz(T[p,q]) = \frac{1}{4}n^2m = \frac{1}{4}(pq)^2\left(\frac{3}{2}(pq)\right) = \frac{3}{8}p^3q^3.$$

To explain our proof in the previous lemma, in what follows we compute the matrix A and X of distances from vertices 1 and 2 in Figure 3. We have:

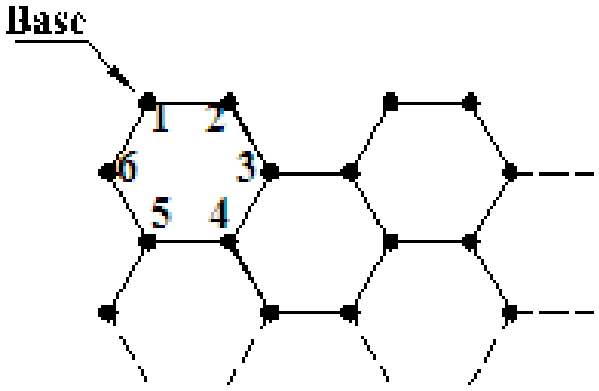

Fig. 3. The Fragment of an Achiral Polyhex Nanotorus.

$$A_{16,16} = \begin{bmatrix}
0 & 1 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\
1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 2 \\
2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\
3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\
4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\
5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\
6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\
7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\
8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\
7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 \\
6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 16 & 15 & 12 & 11 & 10 & 9 & 8 & 7 \\
5 & 6 & 7 & 8 & 9 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 8 & 7 & 6 \\
4 & 5 & 6 & 7 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 6 & 5 \\
3 & 4 & 5 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 4 \\
2 & 3 & 4 & 5 & 8 & 9 & 12 & 13 & 16 & 15 & 12 & 11 & 8 & 7 & 4 & 3 \\
1 & 2 & 3 & 6 & 7 & 10 & 11 & 14 & 15 & 14 & 13 & 10 & 9 & 6 & 5 & 2
\end{bmatrix}$$

$$X_{16,16} = \begin{bmatrix}
1 & 0 & 3 & 4 & 7 & 8 & 11 & 12 & 15 & 16 & 13 & 12 & 9 & 8 & 5 & 4 \\
2 & 1 & 2 & 5 & 6 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 7 & 6 & 3 \\
3 & 2 & 3 & 4 & 7 & 8 & 11 & 12 & 15 & 16 & 13 & 12 & 9 & 8 & 5 & 4 \\
4 & 3 & 4 & 5 & 6 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 7 & 6 & 5 \\
5 & 4 & 5 & 6 & 7 & 8 & 11 & 12 & 15 & 16 & 13 & 12 & 9 & 8 & 7 & 6 \\
6 & 5 & 6 & 7 & 8 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 9 & 8 & 7 \\
7 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 15 & 16 & 13 & 12 & 11 & 10 & 9 & 8 \\
8 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\
9 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 15 & 14 & 13 & 12 & 11 & 10 \\
8 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\
7 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 15 & 16 & 13 & 12 & 11 & 10 & 9 & 8 \\
6 & 5 & 6 & 7 & 8 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 9 & 8 & 7 \\
5 & 4 & 5 & 6 & 7 & 8 & 11 & 12 & 15 & 16 & 13 & 12 & 9 & 8 & 7 & 6 \\
4 & 3 & 4 & 5 & 6 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 7 & 6 & 5 \\
3 & 2 & 3 & 4 & 7 & 8 & 11 & 12 & 15 & 16 & 13 & 12 & 9 & 8 & 5 & 4 \\
2 & 1 & 2 & 5 & 6 & 9 & 10 & 13 & 14 & 15 & 14 & 11 & 10 & 7 & 6 & 3
\end{bmatrix}$$

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