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REVISED SZEGED INDEX OF TC_4C_8(R) NANOTORUS

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ABSTRACT. The revised Szeged index is a recently introduced topological index. In this paper, the revised Szeged index of TC_4C_8(R) nanotorus is computed.

Keywords: *Rhombic TC_4C_8(R) nanotorus, revised Szeged index.*

INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. A topological index is a number invariant under automorphisms of the considered graph.

It is easy to see that the vertex set V(G) equipped with the distance function d_G is a metric space and so the topological indices related to d_G carry important structural information on the molecule under consideration. The Szeged index is one of these topological indices and it was introduced by Ivan Gutman [1]. It is defined as

$$Sz(G) = \sum_{e=uv} n_u(e)n_v(e),$$

where $n_u(e)$ is the number vertices closer to u than v and $n_v(e)$ is defined analogously.

Milan Randić [2] presented a modification of this topological index to find better applications in chemistry. Later this modification was named the revised Szeged index. It is defined as

$$Sz^*(G) = \sum_{e=uv}\left[n_u(e) + \frac{n_0(e)}{2}\right]\times\left[n_v(e) + \frac{n_0(e)}{2}\right],$$

where $n_0(e)$ denotes the number of vertices equidistant from u and v. We refer the reader to [3] for mathematical notations used in this paper. The aim of this paper is to compute the revised Szeged index of a rhombic nanotorus

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R[p,q] depicted in Figure 1. To do this, we first draw the molecular graph of nanotorus by HyperChem [3]. The same can be done by CVNET, by Diudea et al. [4,5]. Then we apply this HIN file to compute adjacency and distance matrix of the given nanotorus by TopoCluj software [6]. Finally, we prepare some programs by the computer algebra system GAP [7] to compute the revised Szeged index of some nanotori. This allowed to find some conjectures on our problem. Our final task is to prove these conjectures and compute the desired topological index.

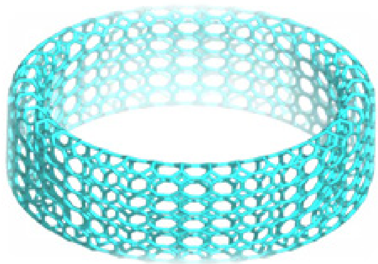

Figure 1. 3D view of $TC_4C_8(R)[p,q]$

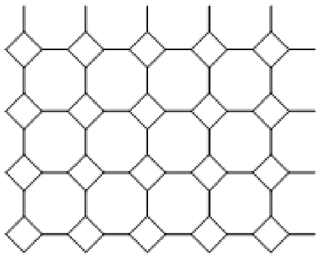

Figure 2. 2D view of R[5,4]

Our notations are taken from a recently published book of Diudea and Nagy [8]. A graph G is called bipartite if its vertex set can be partitioned into subsets A and B in such a way that each edge of G connects a vertex of A to a vertex of B. We encourage to the interested reader to see [9,10] for some applications in physics and chemistry. The aim of this paper is to compute the revised Szeged index of an arbitrary $TC_4C_8(R)[p,q]$ nanotorus, where p is the number of rhombs in each row and q is the number of rhombs in each column. The main result of this paper is the following theorem:

THEOREM: The revised Szeged index of $TC_4C_8(R) = TC_4C_8(R)[p,q]$, p is odd, is computed as follows

$$Sz^*(TC_4C_8(R)) = \begin{cases} 24p^3q^3 & q \text{ is odd} \\ 24p^3q^3 - pq^3 & 2 \mid q \ \& \ q < p \\ 24p^3q^3 - p^3q & 2 \mid q \ \& \ q > p \end{cases}$$

RESULTS AND DISCUSSION

The unit rhombic cell U of the rhomb-octagonal lattice R has been chosen having the four vertices represented in Figure 2. This selection allows the generation of the complete 2–dimensional infinite lattice by pure translational operation along both lattice directions. We denote the obtained lattice by $TUC_4C_8(R)$ and in closed form by $TC_4C_8(R)$.

The aim of this section is to compute the revised Szeged index of an arbitrary $TC_4C_8(R)[p,q]$ nanotorus, when p is odd. To do this we first notice that the Szeged and revised Szeged indices of bipartite graphs are the same. In [11] the Szeged index of $TC_4C_8(R)$ nanotorus was computed in general. In fact, it is proved that the Szeged index of $TC_4C_8(R)$ is equal to $24p^3q^3$. Here we consider the cases that one of p and q are odd. Without loss of generality, we assume that p is odd.

From Figure 2, we can see that it is possible to partition the set of edges into three subsets A, B and C such that A is the set of all horizontal edges, Figure 3(a), B is the set of all vertical edges, Figure 3(b), and C is the set of all edges of rhombs of $TC_4C_8(R)$, Figure 3(c).

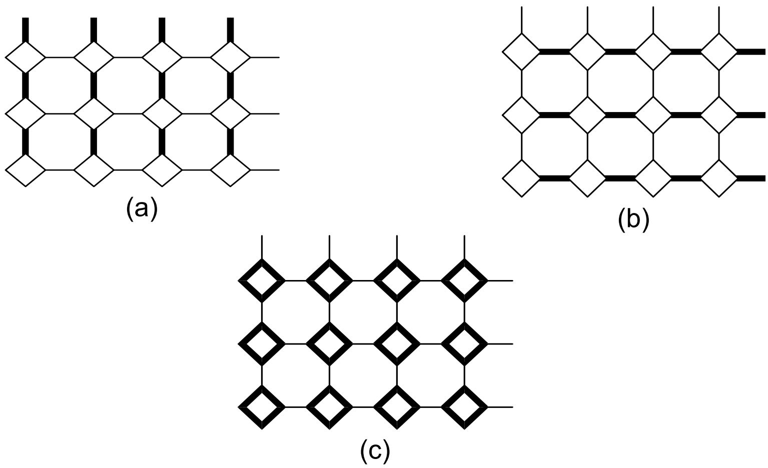

Figure 3. Three Types of Edges in $TC_4C_8(R)$.

For a given q we consider two cases that $p < q$ or $p \geq q$. If q is even then the quantities $n_u(e)$, $n_v(e)$ and $n_0(e)$ for each horizontal, vertical and rhombic edges of $TC_4C_8(R)$ are computed in Table 1. We notice that from the symmetry of $TC_4C_8(R)$ nanotorus these quantities are the same on each element of A. The same is correct for B and C. When q is odd, then it is possible to find an automorphism f of $TC_4C_8(R)$ such that f maps a vertical edge to a rhombic one. This shows that in this case the quantities n_u, n_v and n_0 for vertical and rhombic edges are the same. In Table 1, these quantities are recorded.

Table 1. The number of vertices closer to u than to v, the number of vertices closer to v than to u and equidistant vertices in $TC_4C_8(R)[p,q]$.

The number of vertices closer to u than to v, The number of vertices closer to v than to u and Equidistant vertices	***No of Vertices***	***p,q***
$\begin{cases} 2pq, 2pq, 0 \\ 2pq-2q+p, 2pq-2q+p, 4q-2p \\ 2pq, 2pq-p, p \end{cases}$	$\begin{cases} pq \\ pq \\ 4pq \end{cases}$	$p<q,\ 2\mid q$
$\begin{cases} 2pq, 2pq, 0 \\ 2pq-q, 2pq-q, 2q \\ 2pq, 2pq-q, q \end{cases}$	$\begin{cases} pq \\ pq \\ 4pq \end{cases}$	$p\geq q,\ 2\mid q$
$\begin{cases} 2pq-2p+q, 2pq-2p+q, 4p-2q \\ 2pq-q, 2pq-q, 2q \end{cases}$	$\begin{cases} pq \\ 5pq \end{cases}$	$p \geq q,\ 2\nmid q$
$\begin{cases} 2pq-2q+p, 2pq-2q+p, 4q-2p \\ 2pq-p, 2pq-p, 2p \end{cases}$	$\begin{cases} pq \\ 5pq \end{cases}$	$p<q,\ 2\nmid q$

Also, some values of revised Szeged indices of this nanotorus are computed in Table 2.

Table 2. The revised Szeged indices of $TC_4C_8(R)$ nanotorus for some values of p and q.

p	**q**	**Sz*($TC_4C_8(R)$)**
3	5	81000
5	4	191680
5	6	647250
5	2	23960

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