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ECCENTRIC CONNECTIVITY INDEX OF TOROIDAL FULLERENES

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ABSTRACT. The eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex x of G. The eccentric connectivity index $\xi(G)$ of G is defined as $\xi(G) = \sum_{u \in V(G)} deg(u)\varepsilon(u)$. In this paper a new method is presented by which it is possible to compute the eccentric connectivity index of molecular graphs. We apply our method to compute the eccentric connectivity index of toroidal fullerenes.

Keywords: *Toroidal Fullerene, Eccentric Connectivity index, Topological indices.*

INTRODUCTION

The discovery of C_{60} bucky-ball, which has a nanometer-scale hollow spherical structure in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [1,2]. Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Suppose p, h, n and m are the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is n = (5p + 6h)/3, the number of edges is m = 3/2n = (5p + 6h)/2 and the number of faces is f = p + h. By the Euler's formula n − m + f = 2, one can deduce that (5p + 6h)/3 – (5p + 6h)/2 + p + h = 2, and therefore p = 12, v = 2h + 20 and e = 3h + 30. This implies that such molecules made up entirely of n carbon atoms and having 12 pentagonal and (n/2 − 10) hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20 [3,4].

Let G = (V, E) be a connected bipartite graph with the vertex set V = V(G) and the edge set E = E(G), without loops and multiple edges. Suppose u and v are vertices of G. The distance d(u,v) is defined as the length of a shortest path connecting them. The eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex x of G. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by

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D(G) and the minimum eccentricity among the vertices of G is called radius of G and denoted by R(G). The set of vertices whose eccentricity is equal to the radius of G is called the center of G. It is well known that each tree has either one or two vertices in its center. The eccentric connectivity index $\xi(G)$ of G is defined as $\xi(G) = \sum_{v \in V(G)} deg(v)\varepsilon(v)$ [5-9]. We encourage the reader to consult papers [10-13] for mathematical properties of this new proposed topological index.

RESULTS AND DISCUSSION

In this section, the eccentric connectivity index of a toroidal fullerene is computed [14,15]. To do this, we apply an algebraic approach. Let us recall some definitions and notations. An automorphism of a graph G is a permutation g of the vertex set V(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 G, with the operation of the composition of permutations, is a permutation group on V(G), denoted by Aut(G). Suppose 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 for 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 on X, 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 vertex transitive. It is easily seen that in a vertex transitive graph, degree of vertices are equal and it is denoted by r = r(G). In such a case G is called r-regular. The following simple lemma is crucial in this section. Here our notations are standard and mainly taken from [16-22].

Lemma 1 — Suppose G is a graph, $A_1, A_2, \ldots, A_t$ are the orbits of Aut(G) under its natural action on V(G) and $x_i \in A_i$, $1 \leq i \leq t$. Then $\xi(G) = \sum_{j=1}^{t} |A_j| deg(x_j)\varepsilon(x_j)$. In particular, if G is vertex transitive then $\xi(G) = r(G)|V(G)|\varepsilon(x)$, for every vertex x.

Proof — It is easy to see that if vertices u and v are in the same orbit, then there is an automorphism φ such that $\varphi(u) = v$. Choose a vertex x such that $\varepsilon(u) = d(u,x)$. Since φ is onto, for every vertex y there exists the vertex w such that $y = \varphi(w)$. Thus $d(v,y) = d(\varphi(u), \varphi(w)) = d(u,w)$ and so $\varepsilon(v) = \max\{d(v,y)\}_{y \in V(G)} = \max\{d(u,w)\}_{w \in V(G)} = \varepsilon(u)$. On the other hand, it is a well – known fact that the vertices of a given orbit have equal degrees.

Therefore, $\xi(G) = \sum_{j=1}^{v} |A_j| deg(x_j) \varepsilon(x_j)$ and if G is vertex transitive then $\xi(G) = r(G)|V(G)|\varepsilon(x)$, for every vertex x. This completes our proof.

▲

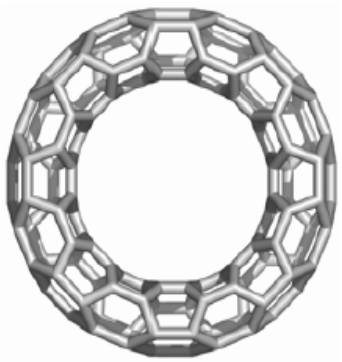

Figure 1. The Zig-zag Polyhex Nanotube.

Apply our method on a toroidal fullerene R = R[p,q], in terms of its circumference (q) and its length (p), Figure 1. To compute the eccentric connectivity index of this fullerene, we first prove its molecular graph is vertex transitive.

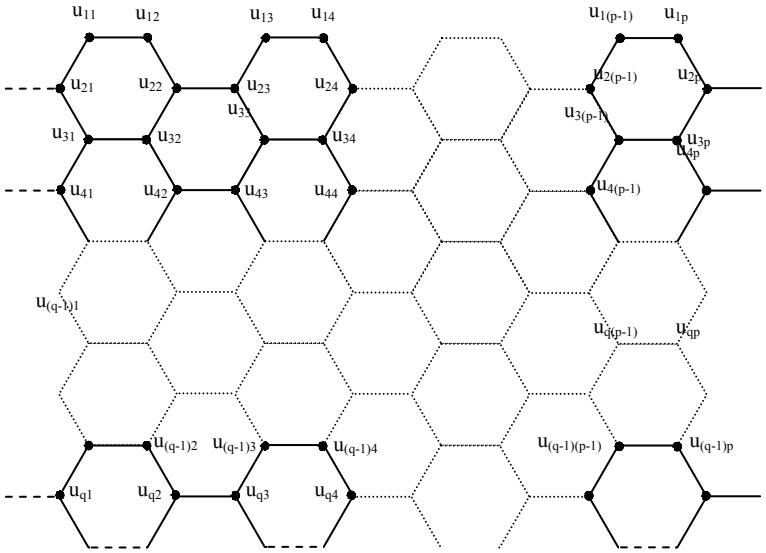

Figure 2. A 2-Dimensional Lattice for T[p,q].

Lemma 2 — The molecular graph of a 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 a polyhex nanotori T = T[p,q], Figure 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}, $1 \leq t \leq p$ and π is a vertical symmetry which maps u_{tj} to u_{ts}, $1 \leq t \leq q$. 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(G), proving the lemma. ▲

Theorem 3 — $\xi(T[p,q]) = 3pq^2$.

Proof — From Figure 2, it can easily seen that $|V(T[p,q])| = pq$. By Lemma 2, T[p,q] is vertex transitive and by Lemma 1, $\xi(T[p,q]) = 3pq\varepsilon(x)$, for a vertex x. Now the proof is follows from this fact that $\varepsilon(x) = q$, proving the result. ▲

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