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COMPUTATION OF ECCENTERIC CONNECTIVITY AND RANDIĆ INDICES OF SOME BENZENOID GRAPHS

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ABSTRACT. Chemical compounds are often modeled as polygonal shapes, where a vertex represents an atom and an edge symbolizes a bond. A topological index is a number related to a molecular graph invariant. In this paper, exact formulas for the eccentricic connectivity and Randić indices of hexagonal parallelogram of benzenoids are given.

Keywords: *Eccentric connectivity, Randić index, hexagonal parallelogram Benzenod, Nanotorus.*

INTRODUCTION

The molecular graph of a molecule *M* is a graph which has atoms of *M* as vertices and two atoms are adjacent if there is a bond between them. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of which being represented by *V(G)* and *E(G)*, respectively.

A topological index is a real number related to a molecular graph, which is a graph invariant. Topological indices have been used extensively for the prediction of physical properties of specific classes of molecules. The oldest topological index is the Wiener index, introduced by Harold Wiener [11].

For vertices $u, v \in V(G)$ the edge connecting *u* and *v* is denoted by *uv* and the distance $d_G(u, v)$ is defined as the length of a shortest path connecting *u* and *v* in *G*. The eccentricity $ecc_G(u)$ is the largest distance between *u* and any other vertex *v* of *G*. We will omit the subscript *G* when the graph is clear from the context. The eccentric connectivity index of the molecular graph *G*, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [10].

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It is defined as: $\xi^c(G) = \sum_{u\in V} d(u)ecc(u)$, where $d(u)$ denotes the degree of the vertex *u* in *G*. We encourage the reader to consult papers [1, 2, 6] for some applications and papers [3-5] for the mathematical properties of this topological index.

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the end vertices of an edge [9]. To preserve rankings of certain molecules, some inequalities involving the weights of edges is needed to be satisfied. Randić [9] stated that weighting all edges *uv* of the associated graph *G* by $(d(u)d(v))^{-1/2}$ preserved these inequalities, where *d(u)* and *d(v)* are the degrees of *u* and *v*. The sum of weights over all edges of *G*, which is called the Randić index, *R(G)*

$$R(G) = \sum_{uv\in E} \frac{1}{\sqrt{d(u)d(v)}}.$$

This index has been closely correlated with many chemical properties [7] and found to parallel the boiling point, Kovats constants, and a calculated surface. In addition, the Randić index appears to predict the boiling points of alkanes more closely, and only it takes into account the bonding or adjacency degree among carbons in alkanes (see [8]).

RESULTS AND DISCUSSION

A graph formed by a row of n hexagonal cells is called an n-hexagonal chain. A hexagonal parallelogram $L_n[G]$, is a graph containing n n-hexagonal chains in every row, see Figure 1. It is clear that $L_n[G]$ has $|V|=2n(n+2)$ and $|E|=3n^2+4n-1$.

In this section, we compute the eccentric connectivity and Randić indices of hexagonal parallelogram $L_n[G]$.

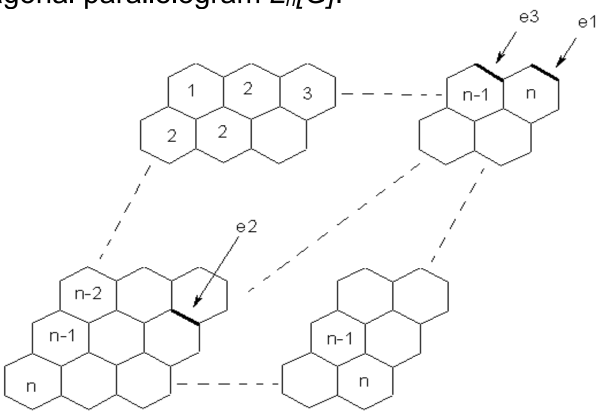

Figure 1. 2-Dimensional graph of a hexagonal parallelogram $L_n[G]$

Theorem 1. The eccentric connectivity index of $L_n[G]$ is

$$\xi^c(L_n[G]) = 24n^3-31n^2+18n-28-\sum_{k=0}^{n-2}(24k^2+k)+\sum_{k=0}^{2n-2}4k \, .$$

Proof. We have for $u \in V(L_n[G])$, *Max* $ecc(u)=4n-1$ and *Min* $ecc(u)=2n$.

In Fig. 2, one can see the eccentricity for every $u \in V(L_n[G])$ while in Fig. 3, one can see several deictic lines for computing the eccentric connectivity index: first line starts with Max $ecc(u)=4n-2$ and finishes with $ecc(u)=2n+1$. The second line starts with $ecc(u)=4n-2$ and finally it has $ecc(u)=2n$. Similarly for another lines we can compute the eccentric connectivity index. Vertices with eccentric connectivity index $4n-1, 4n-2, 4n-4, 4n-6, \ldots, 2n+2, 2n+1$, have $deg(u)=2$ while the other vertices have $deg(u)=3$, where $u \in V(L_n(G))$. Then by using Figs. 2 and 3, we can fill the Table 1, for eccentric connectivity index of the graph.

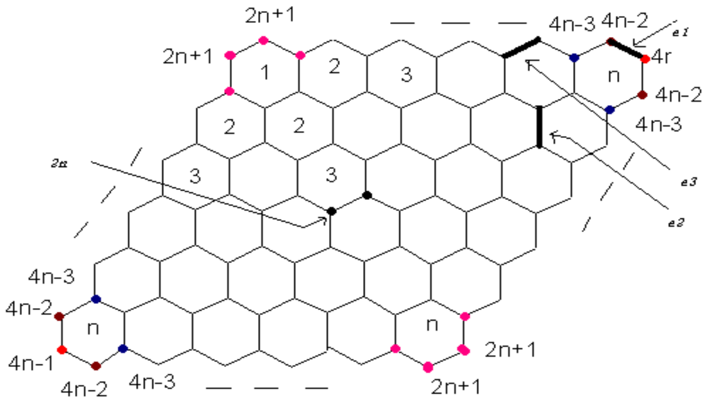

Figure 2. Eccentricity of some vertices $L_n[G]$

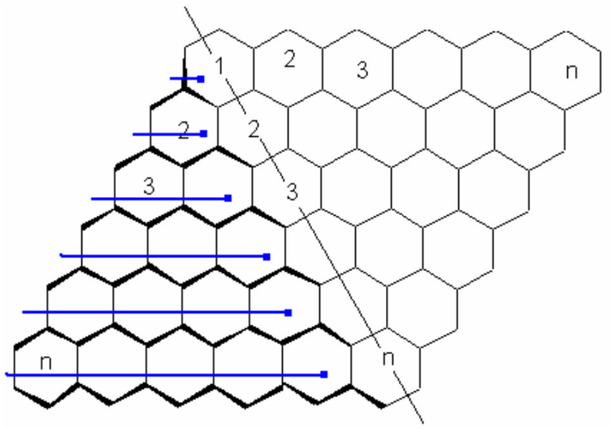

Figure 3. Lines for computing the eccentric connectivity $L_n[G]$

Table 1. Eccentricity of all vertices of $L_n[G]$

Line1	Line2	Line3	Line4	Line5	….	Line(n-1)	Line(n)	ecc
4n-1								max ecc
4n-2	4n-2							
4n-3	4n-3							
4n-4	4n-4	4n-4						
4n-5	4n-5	4n-5	4n-5					
4n-6	4n-6	4n-6	4n-6	4n-6				
4n-7	4n-7	4n-7	4n-7	4n-7				
…..	…..	…..	…..	…..	….			
2n+2	2n+2	2n+2	2n+2	2n+2	….	2n+2		
2n+1	2n+1	2n+1	2n+1	2n+1	….	2n+1	2n+1	
2n+1	2n	2n	2n	2n	….	2n		min ecc

Thus the eccentric connectivity index of hexagonal parallelogram $L_n[G]$ is calculated as follows:

$$\xi^c(L_n[G]) = 2[(4n-1)+2(4n-2)+(4n-3)+(4n-6)+\dots+(2n+3)+(2n+2)+2(2n+1)]$$
$$+6[(n-1)2n+n(2n+1)+5(n-1)+9(n-2)+13(n-3)+\dots+3(4n-11)+2(4n-7)].$$

By arranging the above formula, we have:

$$\xi^c(L_n[G]) = \sum_{k=0}^{n-2} 24(n^2-k^2) + \sum_{k=0}^{n-2}(n-k) + \sum_{k=0}^{2n-2} 4(2n+k) + 20n - 12$$

and next

$$\xi^c(L_n[G]) = 24n^3 - 31n^2 + 18n - 28 - \sum_{k=0}^{n-2}(24k^2+k) + \sum_{k=0}^{2n-2} 4k$$

As it was to be demonstrated.

Theorem 2. The Randić index of $L_n[G]$ is

$$R(L_n[G]) = n^2 - n + 3 - \frac{(n-1)(4\sqrt{6}-1)}{3}.$$

Proof. For computing the Randić index for $L_n[G]$ we consider three type edges, (see fig. 4): (a) edge e_1 with ended vertices of degree 2 and 2, (b) edge e_2 with ended vertices of degree 3 and 3, (c) edge e_3 with ended vertices of degree 2 and 3.

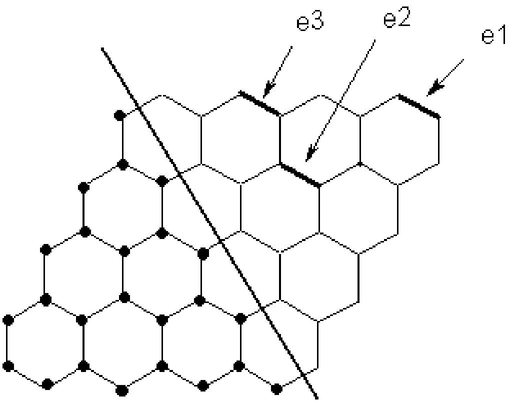

Figure 4. Three type edges e_1**,** e_2 and e_3 of *$L_4[G]$*

It is easy to see that

$$|e_1| = 6,\quad |e_3| = 8(n-1),\qquad |e_2| = (3n-1)(n-1),$$

Thus

$$R(L_n[G]) = \frac{6}{\sqrt{2\times 2}} + \frac{8(n-1)}{\sqrt{2\times 3}} + \frac{(3n-1)(n-1)}{\sqrt{3\times 3}}$$
$$= 3 + \frac{(3n-1)(n-1)}{3} + \frac{4\sqrt{6}(n-1)}{3}.$$

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