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COMPUTING SD-INDEX OF SOME BENZENOID GRAPHS

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Abstract: In this paper, we computed Sd-index of a class of pericondensed benzenoid graph consisting of two rows and having hexagons of various length, for zig-zag and arm chair forms. The results obtained can be generalized further for number of rows.

Keywords: Topological index, Benzenoid graph, Sd-index.

Mathematics Subject Classification: 05C10: Planar graphs; geometric and topological aspects of graph theory, 92E10: Molecular structure (graph-theoretic methods etc.).

1. INTRODUCTION

The graph – theoretical characterization of the molecular structure (molecular graph) is done by its translation into molecular descriptors, called topological indices. A topological index is a numeric quantity from the structural graph of a molecule. Literature survey has indicated that many topological indices have been defined which are used to model chemical, pharmaceutical and other properties of molecules, like, Wiener-, Szeged-, PI-, Sd-, Balaban and Schultz's indices.

Benzenoids (graphical form of benzenoid hydrocarbon) are finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons [6]. Its types are phenylenes and their pericondensed benzenoid graph. These form base of carbon nanostructures like, nanosheets, nanotubes, nanotories etc. A Carbon Nanosheet are carbon nanomaterials formed by one or several monolayers of graphite, where carbon atoms are densely packed in a honeycomb crystal lattice When it is rolled up along certain vectors, it gives rise to different types of nanotubes namely Armchair, Zig-zag and chiral structures. Ashrafi computed the PI index of Benzenoids [1] as well as some nanostructures [2-4]. Both PI-index and Sd-index being cyclic indices, Sd-index could be claimed to be applied to them too.

Sadhana (Sd) Index: In 2006, Khadikar [7] defined the Sd index of a graph G as the sum of edges on both sides of elementary cut i.e.,

$$\text{Sd(G)} = \sum(n_{e_1} + n_{e_2}) \tag{1}$$

where, n_{e1} and n_{e2} are the number of edges on both sides of elementary cut. Similarly, equidistant edges are not counted. In 2009, Aziz and co-workers [5] defined Sadhana (Sd) index mathematically as

$$Sd(G) = m(G)*(c(G) - 1) \tag{2}$$

where G is a sco bipartite graph G (for summation index s = 1, 2, …, c).

2. MAIN RESULT

In this section, Sd-Index for a particular case, of two rows, has been computed for zig-zag and armchair positions in pericondensed benzenoid graphs.

Theorem 1: Prove that the Sd index of a Zig-zag pericondensed benzenoid graph G(m, n), containing two rows, with n and m hexagons respectively, where (m > n) (figure 1) is:

$$Sd(G) = 10m^2 + 6mn + 9m + 3n + 2.$$

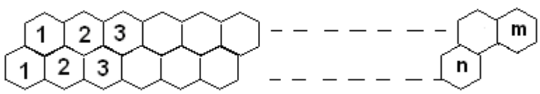

Figure 1: A Zig-zag structure of pericondensed benzenoid graph G(m, n)

Proof: Given, a zig-zag structure of pericondensed benzenoid graph G(m, n), containing two rows (figure 1). On generalizing the sequence of results, by varying the value of n and m, we obtain a general formula for number of edges as m(G) = 5m + 3n + 2 and number of orthogonal cuts as c(G) = 2m + 2. Therefore using equation (2), we get

$$\begin{aligned} Sd(G) &= (5m + 3n + 2)*(2m + 2 - 1) \\ &= 10m^2 + 6mn + 9m + 3n + 2. \text{ Hence proved.} \end{aligned}$$

Theorem 2: Prove that the Sd index of an Armchair pericondensed benzenoid graph (m, n), containing two rows, where m = number of hexagons in a row (in a level) and n = 2 (total no. of rows) respectively (figure 2) is:

$$Sd(G) = 64m^2 + 16mn - 52m - 5n + 10$$

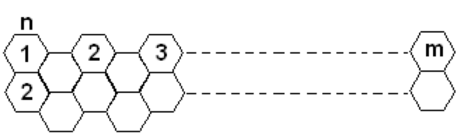

Figure 2: An Armchair structure of pericondensed benzenoid graph G(m, 2)

Proof: Given, an Armchair pericondensed benzenoid graph G(m, 2), containing two rows (figure 2). On generalizing the sequence of results, by varying the value of m, we obtain a general formula for number of edges m(G) = 16m – 5 and number of orthogonal cuts c(G) = 4m + n – 1. Therefore, from equation (2), we get

$$\begin{aligned} Sd(G) &= (16m - 5)*((4m + n - 1) - 1) \\ &= 64m^2 + 16mn - 52m - 5n + 10. \text{ Hence proved.} \end{aligned}$$

3. CONCLUSION

As the Benzenoids forms the base of carbon nanostructures, the results obtained for Sd-index of particular case of two rows can be extended to more different cases and hence general form can be obtained, which is an open problem. The results obtained in our study can be extended to other problems related to computing Sd-index of nanostructures.

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