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The Vertex-Degree of a Molecular Graph

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ABSTRACT: A graph is collection of points and lines connecting a subset of them. The degree of a vertex V of a graph is the number of vertices of G adjacent to V , denoted by d_v . In this paper vertex-degree of molecular graph, molecular graph of molecule $C_{30}H_{18}$, carbon nanotube, fullerenes and carbon nanocones are studied.

KEYWORDS: Molecular graph, topological indices, distance, vertex-degree, carbon nanotube, fullerenes, nanocones.

I. INTRODUCTION

A graph is a mathematical object that consists of two sorts of elements: vertices and edges.

Let $V(G)$ be vertex set and $E(G)$ be the edge set. A molecular graph $G(V, E)$ is constructed by representing each atom of molecule by vertex and bonds between them by edges. One of the oldest graph invariants is the Wiener index $W(G)$, introduced by the chemist Harold Wiener in 1947 [1]. It is defined as the sum of topological distances $d(u, v)$ between any two atoms in the graph G . The distance $d(u, v)$ between the vertices u and v of the graph G is equal to the length of the shortest path that connects u and v . The degree is defined as number of edges with that vertex. The sum of the degrees of the vertices of a graph G is equal to twice the number of edges in G . Number of Odd degree Nodes is even. The maximum degree of any vertex is 4. A topological index of a graph is a number related to graph which is invariant under graph automorphisms [1]. Topological indices are graph invariants, used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies [2]. A loop at v is to be counted twice in computing the degree of v [3]. There are great many degree-based and distance-based topological indices studied in graph theory. A nanostructure is an object of intermediate size for which at least one dimensions is 1nm to 100 nm. The graph of molecule $C_{30}H_{18}$ has hexagonal squeezes which possess only vertices of degree two or three [4]. All graphs considered in this paper are finite, undirected, simple and connected. Molecular graph G of 2, 3-dimethyl hexane with its vertex degrees indicated is given in figure (1) [5]. All the symbols and notations used in this paper are standard and taken mainly from standard books of graph theory [6-10]. The validity of corollary, that In any graph, the number of vertices of odd degree is even is investigated for molecular graphs of 2, 3-dimethyl hexane, $C_{30}H_{18}$, carbon nanotube [1, 12, and 14] and carbon nanocones [13], fullerenes [11]. In this paper vertex-degree of molecular graph, molecular graph of $C_{30}H_{18}$, carbon nanotube, fullerenes and carbon nanocones are studied.

II. MATERIALS AND METHODS

Any connected graph with maximum degree not extending 4 is called molecular graph. A molecular graph is constructed by indicating each atom of a molecule by vertex and bonds connecting atoms by edges. Let G be a simple molecular graph with vertex and edge sets $V(G)$ and $E(G)$ respectively. The number of edges incident with vertex u or the number of vertices adjacent to u is called degree denoted by $d_G(u)$ or $d(u)$. The molecular graph of 2-methyl butane is shown in figure (1). The vertices 1, 4 and 5 are pendent vertices with degree 1. The degree of vertex 2 is 3 and that of 3 is 2. The vertex set $V(G)$ is decided first for 2,3-dimethyl hexane, $C_{30}H_{18}$, carbon nanotubes and fullerenes to compute the vertices with odd and even degrees.

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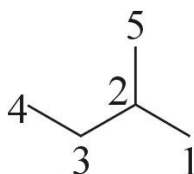


Fig.1. Molecular graph of 2-methylbutane

III. RESULTS AND DISCUSSION

The topological distance $d(u, v)$ is important in graph theory. The degree is defined as the number of edges with that vertex. The maximum degree of any vertex is 4. There is degree-based and distance-based topological indices studied in chemical graph theory. Molecular graph G of 2, 3-dimethyl hexane with its vertex degrees indicated is represented in figure (2). In the molecular graph of 2,3-dimethyl hexane, there are 8 vertices with degrees 1, 2 and 3. The odd degrees are 1 and 3. The number of vertices with odd degrees for 1 and 3 are 4 and 2 respectively. In the molecular graph of $C_{30}H_{18}$ vertices with odd degree are 12 and even degrees are 18. In $HAC_5C_7[p, q]$ carbon nanotube the vertices with odd degree (3) are 56 and vertices with even degree (2) is 10. For Carbon nanocones $C_5(1)$, $C_7(1)$ odd degree vertices are 3 are 10 and 14 respectively. The two dimensional structure of fullerene C_{38} with 38 vertices and 16 cycles is represented in fig.(3) [11]. In fullerenes C_{38} and C_{64} odd degrees are 38 and 64 respectively, no vertex with even degree. In any type of fullerene there is only odd degree due to particular type of locking of cycles

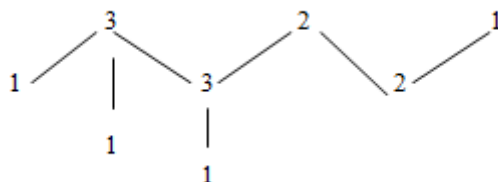


Fig .2. Molecular graph G of 2, 3-dimethyl hexane with its vertex degrees indicated.

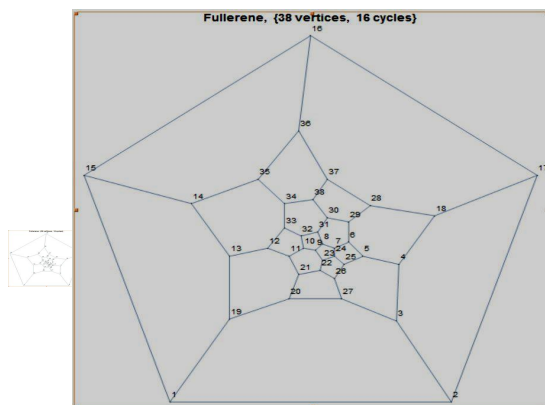


Fig .3. Fullerene with 38 vertices and 16 cycles.

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IV. CONCLUSION

The vertex degree of molecular graphs of molecules and nanostructures are studied. The vertex-degree is important in the computation of degree-based and distance-based topological indices of nanostructures. The odd degrees for molecular graphs are 1 and 3 and even degrees are 2 and 4. In fullerenes C_{38} and C_{64} the degree of each vertex is 3. It is observed that for molecular graph of 2, 3-dimethyl hexane, $C_{30}H_{18}$, Carbon nanotube HC_5C_7 [p, q], fullerenes and carbon nanocones the number of vertices with odd degree is even.

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