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THE GENERAL CONNECTIVITY INDICES OF POLYCYCLIC AROMATIC HYDROCARBONS

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Abstract

The general connectivity index is important one and has more application in physico-chemical science and vice versa. In this paper, we focus on the structures of this Polycyclic Aromatic Hydrocarbons and computing the general connectivity indices of this family of hydrocarbon structures.

Keywords: general connectivity index, polycyclic aromatic hydrocarbons.

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1. Introduction

In physico-chemical science, the structure of a molecule could be represented in a variety of ways. The information on the physico-chemical constitution of molecule is conventionally represented by a molecular graph. And graph theory was successfully provided the physicist and chemist with a variety of very useful tools, namely, topological indices.

Let $G = (V, E)$ be a simple finite molecular graph with the vertex set $V(G)$ and the edge set $E(G)$. In physico-chemical graph theory, the vertices and the edges correspond to the atoms and the bonds, respectively. All other notation and terminology are referred to [1]. The second Zagreb index has been introduced more than forty years ago by Gutman and Trinajestic ([2]), which is defined as

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v).$$

Later, Bollobás and Erdös [3] generalized this index by replacing $-\frac{1}{2}$ with any real number α and it is called the general connectivity index of a molecular $G = (V, E)$ as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

2. Main Results

In this section, we compute the general connectivity index of a family of polycyclic aromatic hydrocarbons as follows. These indices should reflect directly the material natural properties.

For convenience, it is necessary to simplify some basic concepts and notations. An i-vertex denotes a vertex degree i, and m_{jk} be the number of (j, k)-edge, respectively.

Theorem 2.1. *Let PAH_n be the general representation of the polycyclic aromatic hydrocarbons molecules for any positive integer n. Then for any real number α, the general connectivity index is equal to*

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha = 3^{\alpha+1} \cdot n \cdot [3^{\alpha+1} \cdot n + (2 - 3^\alpha)]. \quad (3.1)$$

Proof. By usage of the definitions of the general connectivity index, we can compute it of polycyclic aromatic hydrocarbon PAH_n as follows:

$$R_\alpha(PAH_n) = \sum_{uv \in E(G)} (d_u d_v)^\alpha = m_{13}(1 \times 3)^\alpha + m_{33}(3 \times 3)^\alpha$$

$$= 3^\alpha(6n) + 9^\alpha(9n^2 - 3n) = 3^{\alpha+1} \cdot n \cdot [3^{\alpha+1} \cdot n + (2 - 3^\alpha)].$$

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