GENERAL (α, 2)-PATH SUM-CONNECTIVITY INDICES OF TWO CLASSES OF GRAPHS

Chuantao Li

School of Science, China University of Geosciences (Beijing), Beijing 100083, P. R. China

Abstract

General $(\alpha, 2)$ -path sum-connectivity index of a molecular graph originates from many practical problems such as discovering new drugs. In this paper, we completely compute their values of two classes graphs.

Keywords: general $(\alpha, 2)$ -path sum-connectivity index, path, cycle.

1. Introduction

Topological indices of molecular graphs are very important invariants of molecular graphs, which can be used to explore properties of molecular structured graphs. They have been studied by a lot of scientists both in mathematics and in chemistry for many years. Researchers propose one

^{*}Corresponding author.

E-mail address: 2012010020@cugb.edu.cn (Chuantao Li).

Copyright © 2018 Scientific Advances Publishers 2010 Mathematics Subject Classification: 05C78. Submitted by Fundamental Research Funds for the Central Universities (No. 2652015193 and No. 2652017146). Submitted by Haiying Wang. Received August 15, 2018

new class of topological index, named the general $(\alpha, 2)$ -path sumconnectivity index of a molecular graph. It originates from many practical problems such as three dimensional quantitative structure-activity (3DQSAR), molecular chirality and discovering many new drugs [2].

Let G = (V, E) be a simple molecular graph with the vertex set Vand the edge set E. Denote the numbers of vertices and edges by |V| and |E|, respectively. In physico-chemical graph theory, the vertices and the edges correspond to the atoms and the bonds, respectively. Two vertices uand v are *adjacent* if there exist an edge e = uv between them in G. The number of all adjacent vertices of u is called its *degree*, denoted by d(u). An *i*-vertex denotes a vertex degree *i*. Let $v_{i_0}v_{i_1}v_{i_3}$ be a path P^2 of length 2 in G. Let m_{122} and m_{222} denote the numbers of all 2-paths of the degree sequence types (1, 2, 2) and (2, 2, 2) in G, respectively. Let P_n and C_n denote Path and Cycle with n vertices, respectively. All other notations and terminologies are referred to [1].

With the intention of extending the applicability, we begin to consider *the general* $(\alpha, 2)$ *-path sum-connectivity index* of *G* as where we take the sum over all possible paths of length 2 of *G*

$${}^{2}\chi_{\alpha}(G) = \sum_{P^{2} = v_{i_{1}}v_{i_{2}}v_{i_{3}} \subseteq G} [d(v_{i_{1}}) + d(v_{i_{2}}) + d(v_{i_{3}})]^{\alpha},$$

with any nonzero real number α and any positive integer *t*, and two paths $v_{i_1}v_{i_2}v_{i_3}$ and $v_{i_3}v_{i_2}v_{i_1}$ are considered to be one path.

2. Main Results

In this section, we begin to compute general $(\alpha, 2)$ -path sumconnectivity indices of Path and Cycle.

Theorem 1. ${}^{2}\chi_{\alpha}(P_{n}) = 2 \cdot 5^{\alpha} + (n-3) \cdot 6^{\alpha}$.

Proof. According to the structures of Path P_n , there are in all two different 2-paths, which degree sequences are (1, 2, 2) and (2, 2, 2), respectively. Then $m_{122} = 2$ and $m_{222} = n - 3$ in P_n . Then ${}^2\chi_{\alpha}(P_n) = 2(1+2+2)^{\alpha} + (n-3)(2+2+2)^{\alpha} = 2 \cdot 5^{\alpha} + (n-3) \cdot 6^{\alpha}$.

Theorem 2. ${}^{2}\chi_{\alpha}(C_{n}) = n \cdot 6^{\alpha}$.

Proof. According to the structures of C_n , there are unique type 2-path, which degree sequences is (2, 2, 2). Then $m_{222} = n$. Then ${}^2\chi_{\alpha}(C_n)$ $= n(2+2+2)^{\alpha} = n \cdot 6^{\alpha}$.

References

- J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, MacMillan, New York, NY, 1976.
- [2] L. B. Kier and L. H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.