سیویلیکا - ناشر تخصصی مقالات کنفرانس ها و ژورنال ها
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عنوان مقاله:

COMPUTING SOME TOPOLOGICAL INDICES OF NANO STRUCTURES

محل انتشار:

همایش منطقه ای شیمی (سال: 1389)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Jafar Asadpour - *Islamic Azad University, Miyaneh Branch, Miyaneh, Iran*

Rasol Mojarad - *Islamic Azad University, Bushehr Branch, Bushehr Iran*

Lila Safikhani - *Islamic Azad University, Miyaneh Branch, Miyaneh, Iran*

خلاصه مقاله:

All of the graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted [1]. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [2,3,4]. This theory had an important effect on the development of the chemical sciences. A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin [5]. If x,yV(G) then the distance dG(x,y) between x and y is defined as the length of any shortest path in G connecting x and y. The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [2]. They are defined as (فرمول در متن اصلی مقاله) where du and dv are the degrees of u and v. The connectivity index introduced in 1975 by Milan Randić [3, 4, 5], who has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as follows (فرمول در متن اصلی مقاله) In this paper we compute some topological indices for TUC4C8(S) nanotube.

کلمات کلیدی:

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