Abstract

Graphs of unbranched hexagonal systems consist of hexagonal rings connected with each other. Molecular graphs of unbranched polycyclic aromatic hydrocarbons serve as an example of graphs of this class. The Wiener index (or the Wiener number) of a graph is defined as the sum of distances between all pairs of its vertices. Necessary conditions for the existence of graphs with different numbers of hexagonal rings and equal values of the Wiener index are formulated, and examples of such graphs are presented.

1. Introduction

One of the promising trends of mathematical chemistry is the construction and investigation of molecular graph invariants which could be used to describe structures of chemical compounds. Such invariants, called topological indices, are used to reveal molecular similarity, order isomers, and compare molecular skeleton forms, characterize molecular branching and cycling, establish the relationship between structure and properties of molecules, predict biological activity of chemical compounds, etc. [1–5]. Among a great number of papers on topological indices, two trends are discernible. The papers of the first trend are dedicated to the construction and application of topological indices to particular problems of chemistry. The papers of the second trend deal with the properties of topological indices as mathematical objects. There is a close relationship between the above trends as, on the one hand, a profound mathematical investigation covers the indices which have already shown their advantages in chemical applications and, on the other hand, the mathematical analysis of the index properties provides additional information to a scientist by revealing the features of the indices' behaviour and possible restrictions, thus allowing the use of the indices with a greater comprehension.

The most important characteristic of any topological index is its sensitivity in the process of molecular structure classification. If topological index values coincide for two different molecular graphs, i.e. the index degenerates on these structures,
then it is less sensitive than the index which differentiates these graphs. In problems of compound property prediction, the assumption is often used that molecules with similar structures (or values of the index as a measure of similarity) have similar properties. Thus, the discriminating ability of the index and the structure of graphs where the index degenerates are important for the investigation of topological indices.

The Wiener index (or the Wiener number), which is equal to the sum of distances between all pairs of molecular graph vertices, is one of the most well-known topological indices. For this index and its modifications, the relationship is established between its values and properties of chemical compounds, in particular, polycyclic aromatic structures [6–11].

2. Basic definitions

We consider finite connected graphs without loops and multiple edges; \( V(G) \) is a set of vertices of the graph \( G \) and \( |V(G)| \) is the order of the graph. Define a class of graphs where all internal faces on a plane are hexagonal, and two arbitrary faces either have only a common edge (i.e. they are adjacent), or have no common vertices. Each face is adjacent to no more than two other faces. Hexagonal faces together with their bound are called the rings of the graph. By placing each hexagonal ring in correspondence with a new vertex and then joining them (if the corresponding rings are adjacent), we obtain the characteristic graph of the initial one. A set of graphs consisting of \( h \) rings for which their characteristic graph is isomorphic to a simple path is denoted by \( G_h \). Graphs \( G_1, G_2 \) and \( G_3 \) (see fig. 1) belong to the class \( G_h \).

![Fig. 1.](image)

Graphs of this class model molecular structures of unbranched cata-condensed benzenoid hydrocarbons [12]. The order of any graph from \( G_h \) is obviously equal to \( 4h + 2 \), and all vertices of the graph have degree 2 or 3. By the distance \( d(u, v) \) between vertices \( v, u \in V(G) \) we mean the length of a simple path which joins the vertices \( v \) and \( u \) in the graph \( G \) and contains the minimal number of edges. The Wiener index of the