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Chemical Graph Theory: A Combination of Chemistry and Maths

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INTRODUCTION

Mathematical chemistry's branch of chemical graph theory employs conventional graph theory to investigate chemical phenomena and entities. In chemical graph theory, molecular structures are represented by chemical graphs. In this type of chemical graph, the edges and nodes stand in for atoms and bonds, respectively. Chemcial graphs are the main types of data structures used in cheminformatics to depict chemical structures. The computable features of graphs serve as the basis for (quantitative) structure activity and structure property predictions, a key field in cheminformatics.

DESCRIPTION

Graph-theoretical descriptors or indices that can then be reduced to these graphs can subsequently are used to depict the physical properties of molecules. One of the most well-known instances of a graph-based molecular descriptor is the Wiener index. The total length of all shortest pathways in a molecule is related to the boiling points of that substance. Among the many uses of graph theory in chemistry, some examples include the counting of isomers, looking for molecular substructures in chemical databases, and creating molecular structures. The representation of an atomic structure by a graph with atoms acting as the vertices and bonds acting as the edges is a significant application of (connected undirected) graphs that is the focus of research in the area known as chemical graph theory. The complete (topological) structure of such a graph can be represented by a single integer, known as a chemical index. Chemical characteristics like boiling points or energies are typically connected to these values. The maximum or minimum values of such an index are particularly important for a certain graph topology.

There have been numerous suggestions for these chemical indicators. They are typically represented in spectral graph theory using the vertex degrees, the (topological) distances between the vertices, or the spectra of the matrices characterizing the graph. This book examines the most important of these indices. Although the major concepts and terminologies are introduced right away, a basic understanding of graph theory is not necessary, but it could be advantageous for the reader to be somewhat familiar with the jargon. As a result, the four chapters that follow a brief introduction go into great detail about the Wiener index, the Radi index, the dual Merrifield-Simmons and Hosoya indices, as well as a number of spectral indices.

The standard 0-1 adjacency matrix's analogue, the incidence matrix, is then discussed. Even more exciting is the Laplacian, which is the diagonal matrix less the adjacency matrix. These matrices are symmetric, which makes their spectra real. This is an unproven characteristic of linear algebra. This presupposes that the reader is knowledgeable in these subjects. This spectral analysis provides substantially more choices for studying the graph's attributes than the indices of the earlier chapters. There are, however, a few unforeseen relationships as well. For a graph of n vertices, the Kirchoff index, for example, is equal to 1/n times the sum of the inverses of the non-zero eigen values of the Laplacian. It is the tree-based analogue of the Wiener index.

CONCLUSION

Despite the fact that the text's primary objective is to clarify each concept and property so that it may be used to molecular chemistry, some of them, such as the spectral and energy indices, can also be applied to networks. However, the emphasis of the treatment is on theory and mathematics. Applications and numerical or algorithmic calculations are excluded.

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CONFLICT OF INTEREST

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