

Wiener Index Of A Graph And Chemical Applications

Quantitative studies on structure-activity and structure-property relationships are powerful tools in directed drug research. In recent years, various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors. It has become possible not only to assess diversities or similarities of structure databases, but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly increasing number of compound libraries. They even allow for a controlled de-novo design of new lead structures. This is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day. This practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors. All descriptors are listed with their definition, symbols and labels, formulas, some numerical examples, data and molecular graphs, while numerous figures and tables aid comprehension of the definitions. Cross-references throughout, a list of acronyms and notations allow easy access to the information needed to solve a specific research problem. Examples of descriptor calculations along with tables of descriptor values for a

set of selected reference compounds and an up-to-date reference list add to the practical value of the book, making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers.

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph and can be different structures. In this book, we determine several important topological indices of polynomials of Wiener index of some widely used chemical structures. The present book is an attempt to outline some, certainly not all, mathematical aspects of modern organic chemistry. We have focused our attention on topological, graph-theoretical and group-theoretical features of organic chemistry, Parts A, B and C. The book is directed to all those chemists who use, or who intend to use mathematics in their work, and especially to graduate students. The level of our exposition is adjusted to the mathematical background of graduate students of chemistry and only some knowledge of elementary algebra and calculus is required from the readers of the book. Some less well-known, but still elementary mathematical facts are collected in Appendices 1-4. This, however, does not mean that the mathematical rigor and numerous tedious, but

necessary technical details have been avoided. The authors' intention was to show the reader not only how the results of mathematical chemistry look, but also how they can be obtained. In accordance with this, Part 0 of the book contains a few selected advanced topics which should give the reader the flavour of the contemporary research in mathematical organic chemistry. One of the authors (I.G.) was an Alexander von Humboldt fellow in 1985 when the main part of the book was written. He gratefully acknowledges the financial support of the Alexander von Humboldt Foundation which enabled his stay at the Max-Planck-Institut für Strahlenchemie in Mülheim and the writing of this book.

Graph Theory is a branch of discrete mathematics. It has many applications to many different areas of Science and Engineering. This book provides the most up-to-date research findings and applications in Graph Theory. This book focuses on the latest research in Graph Theory. It provides recent findings that are occurring in the field, offers insights on an international and transnational levels, identifies the gaps in the results, and includes forthcoming international studies and research, along with its applications in Networking, Computer Science, Chemistry, and Biological Sciences, etc. The book is written with researchers and post graduate students in mind.

Originally published in 2001, reissued as part of Pearson's modern classic series.

This contributed volume is inspired by the seminal discovery and identification of C₆₀. Starting with a comprehensive discussion featuring graphene based nanostructures, subsequent chapters include topological descriptions of matrices, polynomials and indices, and an extended analysis of the symmetry and topology of nanostructures. Carbon allotropes such as diamond and its connection to higher-dimensional spaces is explored along with important mathematical and topological considerations. Further topics covered include spontaneous symmetry breaking in graphene, polyhedral carbon structures, nanotube junction energetics, and cyclic polyines as relatives of nanotubes and fullerenes. This book is aimed at researchers active in the study of carbon materials science and technology.

The mathematical combinatorics is a subject that applying combinatorial notion to all mathematics and all sciences for understanding the reality of things in the universe. The International J. Mathematical Combinatorics is a fully refereed international journal, sponsored by the MADIS of Chinese Academy of Sciences and published in USA quarterly, which publishes original research papers and survey articles in all aspects of mathematical combinatorics, Smarandache multi-spaces, Smarandache geometries, non-Euclidean geometry, topology and their applications to other sciences.

The number-one reference on the topic now contains a wealth of new data: The entire relevant literature over the past six years has been painstakingly surveyed, resulting in hundreds of new descriptors being added to the list, and some 3,000 new references in the bibliography section. Volume 1 contains an alphabetical listing of more than 3300 descriptors and related terms for chemoinformatic analysis of chemical compound properties, while the second volume lists over 6,000 references selected from 450 journals. To make the data even more accessible, the introductory section has been completely re-written and now contains several "walk-through" reading lists of selected keywords for novice users.

Topology in Chemistry Discrete Mathematics of Molecules Elsevier

This volume addresses a number of topological themes of direct relevance to chemists. Topological concepts are now regularly applied in wide areas of chemistry including molecular engineering and design, chemical toxicology, the study of molecular shape, crystal and surface structures, chemical bonding, macromolecular species such as polymers and DNA, and environmental chemistry. Currently, the design and synthesis of new drugs and agrochemicals are of especial importance. The book's prime focus is on the role played by topological indices in the description and characterisation of molecular species.

The Wiener index along with a variety of other major topological indices, are discussed with particular reference to the powerful and much used connectivity indices. In this book an international team of leading experts review their respective fields and present their findings. The considerable benefits offered by topological indices in the investigation of chemical problems in science, medicine, and industry are highlighted. The volume records proceedings of the Harry Wiener Memorial Conference on the Role of Topology in Chemistry, held at the University of Georgia in March 2001, and serves as a fitting tribute to the chemical contributions of the late Harry Wiener. Focuses on the role played by topological indices in the description and characterisation of molecular species Records the proceedings of the Harry Weiner Memorial Conference on the Role of Topology in Chemistry, held at the University of Georgia in March 2001 Along with a variety of other major topological indices, the Wiener index is discussed with particular reference to the powerful and much-used connectivity indices Papers on neutrosophic programming, neutrosophic hypersoft set, neutrosophic topological spaces, NeutroAlgebra, NeutroGeometry, AntiGeometry, NeutroNearRings, neutrosophic differential equations, etc. This book provides a timely overview of fuzzy graph theory, laying the foundation for future applications in a broad range of areas. It introduces readers to

fundamental theories, such as Craine's work on fuzzy interval graphs, fuzzy analogs of Marczewski's theorem, and the Gilmore and Hoffman characterization. It also introduces them to the Fulkerson and Gross characterization and Menger's theorem, the applications of which will be discussed in a forthcoming book by the same authors. This book also discusses in detail important concepts such as connectivity, distance and saturation in fuzzy graphs. Thanks to the good balance between the basics of fuzzy graph theory and new findings obtained by the authors, the book offers an excellent reference guide for advanced undergraduate and graduate students in mathematics, engineering and computer science, and an inspiring read for all researchers interested in new developments in fuzzy logic and applied mathematics. The first book devoted exclusively to quantitative graph theory, *Quantitative Graph Theory: Mathematical Foundations and Applications* presents and demonstrates existing and novel methods for analyzing graphs quantitatively. Incorporating interdisciplinary knowledge from graph theory, information theory, measurement theory, and statistical techniques, this book covers a wide range of quantitative-graph theoretical concepts and methods, including those pertaining to real and random graphs such as: Comparative approaches (graph similarity or distance) Graph measures to characterize graphs quantitatively Applications of

graph measures in social network analysis and other disciplines
Metrical properties of graphs and measures
Mathematical properties of quantitative methods or measures in graph theory
Network complexity measures and other topological indices
Quantitative approaches to graphs using machine learning (e.g., clustering)
Graph measures and statistics
Information-theoretic methods to analyze graphs quantitatively (e.g., entropy)
Through its broad coverage, *Quantitative Graph Theory: Mathematical Foundations and Applications* fills a gap in the contemporary literature of discrete and applied mathematics, computer science, systems biology, and related disciplines. It is intended for researchers as well as graduate and advanced undergraduate students in the fields of mathematics, computer science, mathematical chemistry, cheminformatics, physics, bioinformatics, and systems biology.

An in-depth coverage of selected areas of graph theory focusing on symmetry properties of graphs, ideal for beginners and specialists.

This is the first book to focus on the topological index, the Harary index, of a graph, including its mathematical properties, chemical applications and some related and attractive open problems. This book is dedicated to Professor Frank Harary (1921—2005), the grandmaster of graph theory and its applications. It has been written by experts in the field of graph theory and its applications. For a

connected graph G , as an important distance-based topological index, the Harary index $H(G)$ is defined as the sum of the reciprocals of the distance between any two unordered vertices of the graph G . In this book, the authors report on the newest results on the Harary index of a graph. These results mainly concern external graphs with respect to the Harary index; the relations to other topological indices; its properties and applications to pure graph theory and chemical graph theory; and two significant variants, i.e., additively and multiplicatively weighted Harary indices. In the last chapter, we present a number of open problems related to the Harary index. As such, the book will not only be of interest to graph researchers, but to mathematical chemists as well.

The Cambridge Graph Theory Conference, held at Trinity College from 11 to 13 March 1981, brought together top ranking workers from diverse areas of the subject. The papers presented were by invitation only. This volume contains most of the contributions, suitably refereed and revised. For many years now, graph theory has been developing at a great pace and in many directions. In order to emphasize the variety of questions and to preserve the freshness of research, the theme of the meeting was not restricted. Consequently, the papers in this volume deal with many aspects of graph theory, including colouring, connectivity, cycles, Ramsey theory, random graphs, flows, simplicial decompositions and

directed graphs. A number of other papers are concerned with related areas, including hypergraphs, designs, algorithms, games and social models. This wealth of topics should enhance the attractiveness of the volume.

From specialists in the field, you will learn about interesting connections and recent developments in the field of graph theory by looking in particular at Cartesian products—arguably the most important of the four standard graph products. Many new results in this area appear for the first time in print in this book. Written in an accessible way, *Handbook of Product Graphs, Second Edition* examines the dichotomy between the structure of products and their subgraphs. It also features the design of efficient algorithms that recognize products and their subgraphs and explores the relationship between graph parameters of the product and factors. Extensively revised and expanded, the handbook pre

Introduction to Chemical Graph Theory is a concise introduction to the main topics and techniques in chemical graph theory, specifically the theory of topological indices. These include distance-based, degree-based, and counting-based indices. The book covers some of the most commonly used mathematical approaches in the subject. It is also written with the knowledge that chemical graph theory has many connections to different branches of graph theory (such as extremal graph theory, spectral graph theory). The authors wrote the book in an appealing way that attracts people to chemical graph theory. In doing so, the book is an excellent playground and general

reference text on the subject, especially for young mathematicians with a special interest in graph theory. Key Features: A concise introduction to topological indices of graph theory Appealing to specialists and non-specialists alike Provides many techniques from current research About the Authors: Stephan Wagner grew up in Graz (Austria), where he also received his PhD from Graz University of Technology in 2006. Shortly afterwards, he moved to South Africa, where he started his career at Stellenbosch University as a lecturer in January 2007. His research interests lie mostly in combinatorics and related areas, including connections to other scientific fields such as physics, chemistry and computer science. Hua Wang received his PhD from University of South Carolina in 2005. He held a Visiting Research Assistant Professor position at University of Florida before joining Georgia Southern University in 2008. His research interests include combinatorics and graph theory, elementary number theory, and related problems

In the last hundred years benzenoid hydrocarbons have constantly attracted the attention of both experimental and theoretical chemists. In spite of the fact that some of the basic concepts of the theory of benzenoid hydrocarbons have their origins in the 19th and early 20th century, research in this area is still in vigorous expansion. The present book provides an outline of the most important current theoretical approaches to benzenoids. Emphasis is laid on the recent developments of these theories, which can certainly be characterized as a significant advance. Emphasis is also laid on

practical applications rather than on "pure" theory. The book assumes only some elementary knowledge of organic and physical chemistry and requires no special mathematical training. Therefore we hope that undergraduate students of chemistry will be able to follow the text without any difficulty. Since organic and physical chemists are nowadays not properly acquainted with the modern theory of benzenoid molecules, we hope that they will find this book both useful and informative. Our book is also aimed at theoretical chemists, especially those concerned with the "topological" features of organic molecules. The authors are indebted to Dr. WERNER SCHMIDT (Ahrensburg, FRG) for valuable discussions. One of the authors (I. G.) thanks the Royal Norwegian Council for Scientific and Industrial Research for financial support during 1988, which enabled him to stay at the University of Trondheim and write the present book.

Trondheim, July 1989
Ivan Gutman
Sven J. Cyvin

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Chapter 1 Benzenoid Hydrocarbons .

Topological Indices and Related Descriptors in QSAR and QSPAR reviews the state of the art in this field and highlights the important advances in the generation of descriptors calculated directly from the structure of molecules. This long-awaited comprehensive book provides all the necessary information to calculate and use these descriptors for deriving structure-activity and structure-property relationships. Written by leading experts in the field, this book discusses the physicochemical significance, strengths, and weaknesses of these indices and presents numerous examples of

applications. This book will be a valuable reference for anyone involved in the use of QSAR and QSPAR in the pharmaceutical, applied chemical, and environmental sciences. It is also suitable for use as a supplementary textbook on related graduate level courses.

Topological Indices and Related Descriptors in QSAR and QSPR reviews the state of the art in this field and highlights the important advances in the generation of descriptors calculated directly from the structure of molecules. This long-awaited comprehensive book provides all the necessary information to calculate and use these descriptors for deriving structure-activity and structure-property relationships. Written by leading experts in the field, this book discusses the physicochemical significance, strengths, and weaknesses of these indices and presents numerous examples of applications. This book will be a valuable reference for anyone involved in the use of QSAR and QSPR in the pharmaceutical, applied chemical, and environmental sciences. It is also suitable for use as a supplementary textbook on related graduate level courses.

The contemporary literature cites Wiener index as a topological parameter associated with tree-like molecular graphs derived from organic molecular structures. Given a graph G the corresponding Wiener index or total distance $W(G)$ is defined as the sum of the graphic distances reckoned across all possible vertex-pairs of G . Then $W(G)$ of a graph G may be co-related to the physico-chemical properties of an organic compound

represented as G . This book explores some combinatorial and graph theoretic aspects of Wiener index of broad interest to practical Computer Scientists and Mathematicians. Such aspects are considered relevant to the process of drug synthesis and in the identification of lead drug candidates. It may be noted that the study of Wiener index and its variants are current areas of research from the standpoint of Mathematical Chemistry.

This text is an attempt to outline the basic facts concerning Kekulé structures in benzenoid hydrocarbons: their history, applications and especially enumeration. We further point out the numerous and often quite remarkable connections between this topic and various parts of combinatorics and discrete mathematics. Our book is primarily aimed toward organic and theoretical chemists interested in the enumeration of Kekulé structures of conjugated hydrocarbons as well as to scientists working in the field of mathematical and computational chemistry. The book may be of some relevance also to mathematicians wishing to learn about contemporary applications of combinatorics, graph theory and other branches of discrete mathematics. In 1985, when we decided to prepare these notes for publication, we expected to be able to give a complete account of all known combinatorial formulas for the number of Kekulé structures of benzenoid hydrocarbons. This turned out to be a much more difficult task than we initially realized: only in 1986 some 60 new publications appeared dealing with the enumeration of Kekulé structures in benzenoids and closely related topics. In any

event, we believe that we have collected and systematized the essential part of the presently existing results. In addition to this we were delighted to see that the topics to which we have been devoted in the last few years nowadays form a rapidly expanding branch of mathematical chemistry which attracts the attention of a large number of researchers (both chemists and mathematicians).

Spectral Radius of Graphs provides a thorough overview of important results on the spectral radius of adjacency matrix of graphs that have appeared in the literature in the preceding ten years, most of them with proofs, and including some previously unpublished results of the author. The primer begins with a brief classical review, in order to provide the reader with a foundation for the subsequent chapters. Topics covered include spectral decomposition, the Perron-Frobenius theorem, the Rayleigh quotient, the Weyl inequalities, and the Interlacing theorem. From this introduction, the book delves deeper into the properties of the principal eigenvector; a critical subject as many of the results on the spectral radius of graphs rely on the properties of the principal eigenvector for their proofs. A following chapter surveys spectral radius of special graphs, covering multipartite graphs, non-regular graphs, planar graphs, threshold graphs, and others. Finally, the work explores results on the structure of graphs having extreme spectral radius in classes of graphs defined by fixing the value of

a particular, integer-valued graph invariant, such as: the diameter, the radius, the domination number, the matching number, the clique number, the independence number, the chromatic number or the sequence of vertex degrees. Throughout, the text includes the valuable addition of proofs to accompany the majority of presented results. This enables the reader to learn tricks of the trade and easily see if some of the techniques apply to a current research problem, without having to spend time on searching for the original articles. The book also contains a handful of open problems on the topic that might provide initiative for the reader's research. Dedicated coverage to one of the most prominent graph eigenvalues Proofs and open problems included for further study Overview of classical topics such as spectral decomposition, the Perron-Frobenius theorem, the Rayleigh quotient, the Weyl inequalities, and the Interlacing theorem

This book builds on two recently published books by the same authors on fuzzy graph theory. Continuing in their tradition, it provides readers with an extensive set of tools for applying fuzzy mathematics and graph theory to social problems such as human trafficking and illegal immigration. Further, it especially focuses on advanced concepts such as connectivity and Wiener indices in fuzzy graphs, distance, operations on fuzzy graphs involving t-norms, and the application of dialectic synthesis in fuzzy graph theory. Each chapter also discusses a number

of key, representative applications. Given its approach, the book provides readers with an authoritative, self-contained guide to – and at the same time an inspiring read on – the theory and modern applications of fuzzy graphs. For newcomers, the book also includes a brief introduction to fuzzy sets, fuzzy relations and fuzzy graphs.

Graphs, Combinatorics, Algorithms and Applications: The research papers contributed by leading experts in their respective field discusses current areas of research in graph theory such as: Graphoidal covers Hyper graphs Domination in graph Signed graphs Graph labelings and Theoretical computer science This volume will serve as an excellent reference for experts and research scholars working in Graph Theory and related topics.

In this issue, there are 17 papers published: Paper 1: Bertrand curves pair, Smarandache curves Paper 2: Dual Lorentzian space, dual curve, dual curves of constant breadth, Bishop frame. Paper 3: (r, m, k) -regular fuzzy graph. Paper 4: edge-antimagic labeling. Paper 5: Ruled surfaces, curve, geodesic. Paper 6: Quarter-symmetric metric connection. Paper 7: Smarandachely k -signed graph. Paper 8: Common fixed point, rational expression. Paper 9: Smarandachely binding number. Paper 10: Wiener index, quasi-total graph. Paper 11: Transformation graph. Paper 12: Probabilistic bounds on weak and strong total

domination in graphs. Paper 13; Smarandachely quotient cordial labeling. Paper 14: Nonholonomic Frames for Finsler Space. Paper 15: b-chromatic number of graphs. Paper 16: Strong defining numbers in graph. Paper 17: A Report on the Promoter Dr. Linfan Mao of Mathematical Combinatorics by your name.

The Fifth International Conference on Computational Science (ICCS 2005) held in Atlanta, Georgia, USA, May 22-25, 2005 ...

Most, yet not all, chemical substances consist of molecules. The fact that molecules have a 'structure' is known since the middle of the 19th century. Since then, one of the principal goals of chemistry is to establish the relationships between the chemical and physical properties of substance and the structure of the corresponding molecules. Countless results along these lines have been obtained along these lines and presented in different publications in this field.

One group uses so-called topological indices. About 20 years ago, there were dozens of topological indices, but only a few with noteworthy chemical applications. Over time, their numbers have increased enormously. At this moment here is no theory that could serve as a reliable guide for solving this problem. This book is aimed at giving a reasonable comprehensive survey of the present, fin de siècle, state of art theory and practice of topological indices.

A comprehensive introduction to the four standard products of graphs and related

topics Addressing the growing usefulness of current methods for recognizing product graphs, this new work presents a much-needed, systematic treatment of the Cartesian, strong, direct, and lexicographic products of graphs as well as graphs isometrically embedded into them. Written by two leading experts in this rapidly evolving area of combinatorics, *Product Graphs: Structure and Recognition* compiles and consolidates a wealth of information previously scattered throughout the literature, providing researchers in the field with ready access to numerous recent results as well as several new recognition algorithms and proofs. The authors explain all topics from the ground up and make the requisite theory and data structures easily accessible for mathematicians and computer scientists alike. Coverage includes

- * The basic algebraic and combinatorial properties of product graph
- * Hypercubes, median graphs, Hamming graphs, triangle-free graphs, and vertex-transitive graphs
- * Colorings, automorphisms, homomorphisms, domination, and the capacity of products of graphs

Sample applications, including novel applications to chemical graph theory Clear connections to other areas of graph theory Figures, exercises, and hundreds of references

This book provides readers with an introduction to m -polar fuzzy graphs and m -polar fuzzy hypergraphs, covering both theories and applications. A special

emphasis is given to m -polar fuzzy graphs at the aim of filling a gap in the literature, namely the absence of a mathematical approach to analyze multi-index, multipolar, and multi-attribute data. The book describes metrics and labeling in m -polar graphs, m -polar fuzzy matroids. It also discusses in detail important applications in decision-making problems and imaging processing. The book is expected to stimulate the curiosity of mathematics, computer scientists, and social scientists alike, and to provide both students and researchers with the necessary knowledge to understand and apply m -polar fuzzy graph theory. In the world of mathematics and computer science, technological advancements are constantly being researched and applied to ongoing issues. Setbacks in social networking, engineering, and automation are themes that affect everyday life, and researchers have been looking for new techniques in which to solve these challenges. Graph theory is a widely studied topic that is now being applied to real-life problems. The Handbook of Research on Advanced Applications of Graph Theory in Modern Society is an essential reference source that discusses recent developments on graph theory, as well as its representation in social networks, artificial neural networks, and many complex networks. The book aims to study results that are useful in the fields of robotics and machine learning and will examine different engineering issues that are closely related to fuzzy graph

theory. Featuring research on topics such as artificial neural systems and robotics, this book is ideally designed for mathematicians, research scholars, practitioners, professionals, engineers, and students seeking an innovative overview of graphic theory.

Graph theory is an important area of applied mathematics with a broad spectrum of applications in many fields. This book results from a Special Issue in the journal Mathematics entitled "Graph-Theoretic Problems and Their New Applications". It contains 20 articles covering a broad spectrum of graph-theoretic works that were selected from 151 submitted papers after a thorough refereeing process. Among others, it includes a deep survey on mixed graphs and their use for solutions to scheduling problems. Other subjects include topological indices, domination numbers of graphs, domination games, contraction mappings, and neutrosophic graphs. Several applications of graph theory are discussed, e.g., the use of graph theory in the context of molecular processes.

A lively invitation to the flavor, elegance, and power of graph theory. This mathematically rigorous introduction is tempered and enlivened by numerous illustrations, revealing examples, seductive applications, and historical references. An award-winning teacher, Russ Merris has crafted a book designed to attract and engage through its spirited exposition, a rich assortment of well-

chosen exercises, and a selection of topics that emphasizes the kinds of things that can be manipulated, counted, and pictured. Intended neither to be a comprehensive overview nor an encyclopedic reference, this focused treatment goes deeply enough into a sufficiently wide variety of topics to illustrate the flavor, elegance, and power of graph theory. Another unique feature of the book is its user-friendly modular format. Following a basic foundation in Chapters 1-3, the remainder of the book is organized into four strands that can be explored independently of each other. These strands center, respectively, around matching theory; planar graphs and hamiltonian cycles; topics involving chordal graphs and oriented graphs that naturally emerge from recent developments in the theory of graphic sequences; and an edge coloring strand that embraces both Ramsey theory and a self-contained introduction to Pólya's enumeration of nonisomorphic graphs. In the edge coloring strand, the reader is presumed to be familiar with the disjoint cycle factorization of a permutation. Otherwise, all prerequisites for the book can be found in a standard sophomore course in linear algebra. The independence of strands also makes Graph Theory an excellent resource for mathematicians who require access to specific topics without wanting to read an entire book on the subject.

Graph-Theoretical Matrices in Chemistry presents a systematic survey of graph-

theoretical matrices and highlights their potential uses. This comprehensive volume is an updated, extended version of a former bestseller featuring a series of mathematical chemistry monographs. In this edition, nearly 200 graph-theoretical matrices are included. This second edition is organized like the previous one—after an introduction, graph-theoretical matrices are presented in five chapters: The Adjacency Matrix and Related Matrices, Incidence Matrices, The Distance Matrix and Related Matrices, Special Matrices, and Graphical Matrices. Each of these chapters is followed by a list of references. Among the matrices presented several are novel and some are known only to a few. The properties and potential usefulness of many of the presented graph-theoretical matrices in chemistry have yet to be investigated. Most of the graph-theoretical matrices presented have been used as sources of molecular descriptors usually referred to as topological indices. They are particularly concerned with a special class of graphs that represents chemical structures involving molecules. Due to its multidisciplinary scope, this book will appeal to a broad audience ranging from chemistry and mathematics to pharmacology.

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