Wiener Index Of A Graph And Chemical Applications

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.

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

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.

The Mathematics and Topology of Fullerenes presents a comprehensive overview of scientific and technical innovations in theoretical and experimental studies. Topics included in this multi-author volume are: Clar structures for conjugated nanostructures; counting polynomials of fullerenes; topological indices of fullerenes; the wiener index of nanotubes; toroidal fullerenes and nanostars; C60 Structural relatives: a topological study; local combinatorial characterization of fullerenes; computation of selected topological indices of C60 and C80 Fullerenes via the Gap Program; 4valent- analogues of fullerenes; a detailed atlas of Kekule structures of C60. The Mathematics and Topology of Fullerenes is targeted at advanced graduates and researchers working in carbon materials, chemistry and physics.

This volume presents some of the research topics discussed at the 2014-2015 Annual Thematic Program Discrete Structures: Analysis and Applications at the Institute for Mathematics and its Applications during Fall 2014, when combinatorics was the focus. Leading experts have written surveys of research problems, making state of the art results more conveniently and widely available. The three-part structure of the volume reflects the three workshops held during Fall 2014. In the first part, topics on extremal and probabilistic combinatorics are

presented; part two focuses on additive and analytic combinatorics; and part three presents topics in geometric and enumerative combinatorics. This book will be of use to those who research combinatorics directly or apply combinatorial methods to other fields.

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

The papers in this volume were presented at the 9th Annual International C- puting and Combinatorics Conference (COCOON 2003), held July 25–28, 2003, in Big Sky, MT, USA. The topics cover most aspects of theoretical computer science and combinatorics related to computing.

Submissionstotheconferencethisyearwereconductedelectronically.Atotal of 114 papers were submitted, of which 52 were accepted. The papers were evaluated by an international program committee consisting of Nina Amenta, Tetsuo Asano, Bernard Chazelle, Zhixiang Chen, Francis Chin, Kyung-Yong Chwa, Robert Cimikowski, Anne Condon, Michael Fellows, Anna Gal, Michael Hallett,DanielHuson,NaokiKatoh,D.T.Lee,BernardMoret,BrendanMumey, Gene Myers, Hung Quang Ngo, Takao Nishizeki, Cindy Phillips, David Sanko?, Denbigh Starkey, Jie Wang, Lusheng Wang, Tandy Warnow and Binhai Zhu. It is expected that most of the accepted papers will appear in a more complete form in scienti?c journals. The submitted papers were from Canada (6), China (7), Estonia (1), F- land (1), France (1), Germany (8), Israel (4), Italy (1), Japan (11), Korea (22), Kuwait (1), New Zealand (1), Singapore (2), Spain (1), Sweden (2), Switzerland (3), Taiwan (7), the UK (1) and the USA (34). Each paper was evaluated by at least three Program Committee members, assisted in some cases by subre- rees. In addition to selected papers, the conference also included three invited presentations by Jon Bentley, Dan Gus?eld and Joel Spencer.

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 contniutions, 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.

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.

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.

How to compute the Wiener index of a graphTopology in ChemistryDiscrete Mathematics of MoleculesElsevier

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.

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.

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 mathe matics 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 mathe matical 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 fUr Strahlenchemie in M iilheim and the writing of this book.

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

This book introduces the study of algebra induced by combinatorial objects called directed graphs. These graphs are used as tools in the analysis of graph-theoretic problems and in the characterization and solution of analytic problems. The book presents recent research in operator algebra theory connected with discrete and combinatorial mathematical objects. It also covers tools and methods from a variety of mathematical areas, including algebra, operator theory, and combinatorics, and offers numerous applications of fractal theory, entropy theory, K-theory, and index theory.

Graph theory is an important area of applied mathematics with a broad spectrum of applications in many fields. This book results from aSpecialIssue 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 ti 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.

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.

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

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 be 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 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.

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.

This book includes papers on the recent advances in state-of-the-art computational science and computing presented at the 2018 International Symposium on Computational Science and Computing (ISCSC 2018), held in Huangshan, China, from

28 to 29 July 2018. All the papers were rigorously peer-reviewed by experts in the area. It is a valuable resource for researchers, professors, graduate students, as well as R & D staff in the industry with a general interest in computational science and computing.
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.
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.
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.
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 ofproduct graph * Hypercubes, median graphs, Hamming graphs, triangle-free graphs, and vertex-transitive graphs * Colorings, automorphisms, homorphisms, 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

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.

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.

Papers on neutrosophic programming, neutrosophic hypersoft set, neutrosophic topological spaces, NeutroAlgebra, NeutroGeometry, AntiGeometry, NeutroNearRings, neutrosophic differential equations, etc.

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

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

The study of topological indices based on distance in a graph in biological sciences, physical - chemistry and QSAR and QSPR studies started from 1947 when Harold Wiener introduced the Wiener index to establishing the relationships between physico-chemistry properties of alkenes and the structures of their molecular graphs. Recent progresses in nano technology caused more attention in calculating topological indices of important molecular graphs such as nanotubes, nanocones and fullerenes. In this monograph, we present an algorithm for computing topological indices based on distance in a graph. By the algorithm the distance between all pairs of vertices is determined and then distance-based topological indices of a graph can be computed. The proposed algorithm is applied to computing the six topological indices: Wiener index, reverse Wiener index, edge Wiener index, eccentric connectivity index, Szeged index and Padmakar-Ivan index for some family of nano structures. Finally, some topological indices such as the Wiener index, the Szeged index, the edge Wiener index, eccentric connectivity index, additively harary index are investigated under some graph operations.

A lively invitation to the flavor, elegance, and power of graphtheory This mathematically rigorous introduction is tempered and enlivenedby numerous illustrations, revealing examples, seductiveapplications, and historical references. An award-winning teacher,Russ Merris has crafted a book designed to attract and engagethrough its spirited exposition, a rich assortment of well-chosenexercises, and a selection of topics that emphasizes the kinds ofthings that can be manipulated, counted, and pictured. Intendedneither to be a comprehensive overview nor an encyclopedicreference, this focused treatment goes deeply enough into asufficiently wide variety of topics to illustrate the flavor,elegance, and power of graph theory. Another unique feature of the book is its user-friendly modularformat. Following a basic foundation in Chapters 1-3, the remainderof the book is organized into four strands that can be exploredindependently of each other. These strands center, respectively,around matching theory; planar graphs and hamiltonian cycles;topics involving chordal graphs and oriented graphs that naturallyemerge from recent developments in the theory of graphic sequences;and an edge coloring strand that embraces both Ramsey theory and aself-contained introduction to Pólya's enumeration ofnonisomorphic graphs. In the edge coloring strand, the reader ispresumed to be familiar with the disjoint cycle factorization of apermutation. Otherwise, all prerequisites for the book can be foundin a standard sophomore course in linear algebra. The independence of strands also makes Graph Theory an excellentresource for mathematicians who require access to specific topicswithout wanting to read an entire book on the subject.

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.

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,

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.