



Wiener Index Of A Graph And Chemical Applications

Ian Pickup



Wiener Index Of A Graph And Chemical Applications:

Introduction to Chemical Graph Theory Stephan Wagner, Hua Wang, 2018-09-05 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 Harary Index of a Graph Kexiang Xu, Kinkar Ch. Das, Nenad Trinajstić, 2015-01-12 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

Quantitative Graph Theory Matthias Dehmer, Frank Emmert-Streib, 2014-10-27 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

Molecular Descriptors for Chemoinformatics

Roberto Todeschini, Viviana Consonni, 2009-10-30 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

The Mathematics and Topology of Fullerenes Franco Cataldo, Ante Graovac, Ottorino Ori, 2011-12-01

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

Discrete Mathematics and Symmetry

Angel Garrido, 2020-03-05 Some of the most beautiful studies in Mathematics are related to Symmetry and Geometry For this reason we select here some contributions about such aspects and Discrete Geometry As we know Symmetry in a system means invariance of its elements under conditions of transformations When we consider network structures symmetry means invariance of adjacency of nodes under the permutations of node set The graph isomorphism is an equivalence relation on the set of graphs Therefore it partitions the class of all graphs into equivalence classes The underlying idea of isomorphism is that some objects have the same structure if we omit the individual character of their components A set of graphs isomorphic to each other is denominated as an isomorphism class of graphs The automorphism of a graph will be an isomorphism from G

onto itself The family of all automorphisms of a graph G is a permutation group Computational Science -- ICCS 2005 V.S. Sunderam, G. Dick van Albada, Peter M.A. Sloot, Jack Dongarra, 2005-05-04 The Fifth International Conference on Computational Science ICCS 2005 held in Atlanta Georgia USA May 22 25 2005 Computing and Combinatorics Tandy Warnow, 2003-07-09 The papers in this volume were presented at the 9th Annual International Computing 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 A total 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 Daniel Huson Naoki Katoh D T Lee Bernard Moret Brendan Mumey 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 scientific journals The submitted papers were from Canada 6 China 7 Estonia 1 Finland 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 subreviewers In addition to selected papers the conference also included three invited presentations by Jon Bentley Dan Gusfield and Joel Spencer

Handbook of Molecular Descriptors Roberto Todeschini, Viviana Consonni, 2008-07-11 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 *Topological Indices and Related Descriptors in QSAR and QSPAR* James Devillers, Alexandru T Balaban, 2000-03-09 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 Modelling of Nanostructures and Extended Systems Ali Reza Ashrafi, Franco Cataldo, Ali Iranmanesh, Ottorino Ori, 2013-05-19 Topological Modelling of Nanostructures and Extended Systems completes and expands upon the previously published title within this series The Mathematics and Topology of Fullerenes Vol 4 2011 by gathering the latest research and advances in materials science at nanoscale It introduces a new speculative area and novel concepts like topochemical reactions and colored reactive topological indices and provides a better understanding of the physical chemical behaviors of extended systems Moreover a charming new family of space filling fullerenic crystals is here analyzed for the first time Particular attention is given to the fundamental influences exercised by long range connectivity topological mechanisms on the chemical and physical properties of carbon nanostructures Systems consisting in graphenic layers with structural and topological defects are investigated in their electronic and magnetic behaviors also in presence of metallic particles More specifically the book focuses on Electronic Properties of low dimensional nanostructures including negatively curved carbon surfaces Pariser Parr Pople model hamiltonian approach to graphene studies Topochemistry and Toporeactivity of extended sp² nanocarbons PAH fullerenes nanoribbons Moebius like nanoribbons nanotubes and grapheme Novel class of crystal networks arising from spanning fullerenes Nanostructures and eigenvectors of matrices and an extended treatise of topological invariants Enumeration hetero fullerenes by Polya theory Topological Modelling of Nanostructures and Extended Systems represents a valuable resource to advances graduates and researchers working in mathematics chemistry physics and material science

Algorithms and Data Structures Pat Morin, Subhash Suri, 2023-07-27 This book constitutes the refereed proceedings of the 18th International Symposium on Algorithms and Data Structures WADS 2023 held during July 31 August 2 2023 The 47 regular papers presented in this book were carefully reviewed and selected from a total of 92 submissions They present original research on the theory design and application of algorithms and data structures

Topology in Chemistry D H Rouvray, R B King, 2002-04-01 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 Wiener 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

Graph-Theoretic Problems and Their New Applications Frank Werner, 2020-05-27 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

Theoretical and Computational Chemistry Editor's Pick 2024, 2nd edition Sam P. De Visser, Thomas S. Hofer, 2025-03-31 We are pleased to introduce the collection Frontiers in Chemistry Theoretical and Computational Chemistry Editor's Pick 2024 This collection showcases most well received spontaneous articles from the past couple of years and have been specially handpicked by our Chief Editors The work presented here highlights the broad diversity of research performed across the section and aims to put a spotlight on the main areas of interest All research presented here displays strong advances in theory experiment and methodology with applications to compelling problems This collection aims to further support Frontiers strong community by recognizing highly deserving authors

Networked Systems Andreas Podelski, François Taïani, 2019-01-05 This book constitutes the thoroughly refereed conference proceedings of the 6th International Conference on Networked Systems NETYS 2018 held in Essaouira Morocco in May 2018 The 22 full and 6 short papers presented together with 11 keynotes and 2 invited papers were carefully reviewed and selected from 85 submissions They are organized in the following topics distribution concurrency verification networking self stabilization security graph and middleware

Recent Trends in Graph Theory & Combinatorics Dr. K.S. Lakshmi, Dr. M.S. Malathy, Dr. S. Indira, Dr. R.A. Lukshmi, 2017-04-07 The seminar was conducted to highlight the vital role of GRAPH THEORY COMBINATORICS in developing mathematical theories for technological

advancement and industrial innovation to bridge the gap between academia and industry to provide a platform for sharing the knowledge of the experts in the field among young students and researchers Distance, Symmetry, and Topology in Carbon Nanomaterials Ali Reza Ashrafi, Mircea V. Diudea, 2016-08-16 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 polyynes as relatives of nanotubes and fullerenes This book is aimed at researchers active in the study of carbon materials science and technology Graph-Theoretical Matrices in Chemistry Dusanka Janezic, Ante Milicevic, Sonja Nikolic, Nenad Trinajstić, 2015-04-22 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 sec **New Frontiers in Nanochemistry: Concepts, Theories, and Trends** Mihai Putz, 2020-05-06 New Frontiers in Nanochemistry Concepts Theories and Trends Volume 2 Topological Nanochemistry is the second of the new three volume set that explains and explores the important basic and advanced modern concepts in multidisciplinary chemistry Under the broad expertise of the editor this second volume explores the rich research areas of nanochemistry with a specific focus on the design and control of nanotechnology by structural and reactive topology The objective of this particular volume is to emphasize the application of nanochemistry With 46 entries from eminent international scientists and scholars the content in this volume spans concepts from A to Z from entries on the atom bond connectivity index to the Zagreb indices from connectivity to vapor phase epitaxy and from fullerenes to topological reactivity and much more The definitions within the text are accompanied by brief but comprehensive explicative essays as well as figures tables etc providing a holistic understanding of the concepts presented

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