



DIMACS

Series in Discrete Mathematics
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Volume 51

Discrete Mathematical Chemistry

DIMACS Workshop
Discrete Mathematical Chemistry
March 23–24, 1998
Rutgers University

Pierre Hansen
Patrick Fowler
Maolin Zheng
Editors



American Mathematical Society

Discrete Mathematical Chemistry

WJ Hussar



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Discrete Mathematical Chemistry Pierre Hansen, P. W. Fowler, Maolin Zheng, 2000 Twenty nine papers from the March 1998 workshop connect issues between chemistry discrete mathematics and computer science Participants discussed theoretical problems of chemistry expressed by discrete mathematics chemical graph algorithms coding theory applied to chemistry applications of discrete mathematics in the chemical industry open problems and directions for research in discrete mathematical chemistry and software for discrete mathematical chemistry Specific topics include isomorphism rejection in structure generation programs fast embeddings for planar molecular graphs geometric symmetry and chemical equivalence and numerical solution of the Laplace equation in chemical space Annotation copyrighted by Book News Inc Portland OR

Advances in Mathematical Chemistry and Applications Subhash C. Basak, Guillermo Restrepo, José L. Villaveces, 2015-10-10 *Advances in Mathematical Chemistry and Applications* Volume 1 highlights the emerging discipline of mathematical chemistry or more precisely discrete mathematical chemistry This Volume is written by internationally renowned experts in the field It comprises of a wise integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery bioinformatics chemoinformatics computational biology and ecological health The contents of this book include chapters on mathematical structural descriptors of molecules and biomolecules topological representation of molecular structure connectivity matrices use of weighted 2D Fingerprints in similarity based virtual screening and much more This ebook is a valuable resource for MSc and PhD students academic personnel and researchers seeking updated and critically important information on the fundamental concepts of mathematical chemistry and their applications

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

Advances in Mathematical Chemistry and Applications: Volume 2 Subhash C. Basak,Guillermo Restrepo,Jose L. Villaveces,2016-02-11 Advances in Mathematical Chemistry and Applications highlights the recent progress in the emerging discipline of discrete mathematical chemistry Editors Subhash C Basak Guillermo Restrepo and Jose Luis Villaveces have brought together 27 chapters written by 68 internationally renowned experts in these two volumes Each volume comprises a wise integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery bioinformatics chemoinformatics computational biology mathematical proteomics and ecotoxicology Volume 2 explores deeper the topics introduced in Volume 1 with numerous additional topics such as topological approaches for classifying fullerene isomers chemical reaction networks discrimination of small molecules using topological molecular descriptors GRANCH methods for the mathematical characterization of DNA RNA and protein sequences linear regression methods and Bayesian techniques in silico toxicity prediction methods drug design integration of bioinformatics and systems biology molecular docking and molecular dynamics metalloenzyme models protein folding models molecular periodicity generalized topologies and their applications and many more Brings together both the theoretical and practical aspects of the fundamental concepts of mathematical chemistry Covers applications in diverse areas of physics chemistry drug discovery predictive toxicology systems biology chemoinformatics and bioinformatics About half of the book focuses primarily on current work new applications and emerging approaches for the mathematical characterization of essential aspects of molecular structure while the other half describes applications of structural approach to new drug discovery virtual screening protein folding predictive toxicology DNA structure and systems biology

Advances in Mathematical Chemistry Subhash C. Basak,Guillermo Restrepo,Jose L. Villaveces,2014-01-01 Advances in Mathematical Chemistry and Applications Volume 1 highlights the emerging discipline of mathematical chemistry or more precisely discrete mathematical chemistry This Volume is written by internationally renowned experts in the field It comprises of a wise integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery bioinformatics chemoinformatics computational biology and ecological health The contents of this book include chapters on mathematical structural descriptors of molecules and biomolecules topological representation of molecular structure connectivity matrices use of weighted 2D Fingerprints in similarity based virtual screening and much more This ebook is a valuable resource for MSc and PhD students academic personnel and researchers seeking updated and critically important information on the fundamental concepts of mathematical chemistry and their applications

Applied Graph Theory and Discrete Mathematics in Chemistry University of Saskatchewan. Mathematical Chemistry Research Unit,1993

Mathematical Chemistry and Chemoinformatics Adalbert Kerber,Reinhard Laue,Markus Meringer,Christoph Rücker,Emma Schymanski,2013-12-12 More than 20 years of experience in molecular structure generation from

conceptualization through to applications Innovative interdisciplinary text demonstrating example queries with software packages such as MOLGEN online Detailed explanations on establishing QSPRs and QSARs as well as structure elucidation using mass spectrometry and structure generation Aims and Scope This work provides an introduction to mathematical modeling of molecules and the resulting applications structure generation structure elucidation QSAR QSPR etc Most chemists have experimented with some software that represents molecules in an electronic form and such models and applications are of increasing interest in diverse and growing fields such as drug discovery environmental science and metabolomics Furthermore structure generation remains the only way to systematically create molecules that are not yet present in a database This book starts with the mathematical theory behind representing molecules explaining chemical concepts in mathematical terms and providing exercises that can be completed online The later chapters cover applications of the theory with detailed explanations on QSPR and QSAR investigations and finally structure elucidation combining mass spectrometry and structure generation This book is aimed in particular at the users of structure generation methods and corresponding techniques but also for those interested in teaching and learning mathematical chemistry and for software designers in chemoinformatics

Solved and Unsolved Problems of Structural Chemistry Milan Randic, Marjana Novic, Dejan Plavsic, 2016-04-21 *Solved and Unsolved Problems of Structural Chemistry* introduces new methods and approaches for solving problems related to molecular structure It includes numerous subjects such as aromaticity one of the central themes of chemistry and topics from bioinformatics such as graphical and numerical characterization of DNA proteins and proteomes It a

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

Essays in the Philosophy of Chemistry Eric Scerri, Grant Fisher, 2016-04-10 The

philosophy of chemistry has emerged in recent years as a new and autonomous field within the Anglo American philosophical tradition With the development of this new discipline Eric Scerri and Grant Fisher s *Essays in Philosophy of Chemistry* is a timely and definitive guide to all current thought in this field One of the themes of this collection is how philosophy of chemistry can make a contributions to problems of philosophy more generally such as how chemistry and quantum chemistry contribute to the philosophy of the mind *Applied Graph Theory and Discrete Mathematics in Chemistry* ,1993

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 *Mathematical Reviews* ,2001 *Applied Graph Theory and Discrete Mathematics in Chemistry* ,1993 *Applied graph theory and discrete mathematics in chemistry* ,1993

Match ,2009 **New Developments in Molecular Chirality** Paul G. Mezey,1991-01-31 Molecular chirality is one of the fundamental aspects of chemistry Chirality properties of molecules have implications in a wide variety of subjects ranging from the basic quantum mechanical properties of simple of a few atoms to molecular optical activity asymmetric synthesis systems and the folding pattern of proteins Chirality in both the geometrical and the topological sense has also been the subject of investigations in various branches of mathematics In particular new developments in a branch of topology called knot theory as well as in various branches of discrete mathematics have led to a novel perspective on the topological aspects of molecular chirality Some of the mathematical advances have already found applications to the interpretation of new concepts in theoretical chemistry and mathematical chemistry as well as to novel synthetic approaches leading to new molecules of exceptional structural properties Some of the new developments in molecular chirality have been truly

fundamental to the theoretical understanding and to the actual practice of many aspects of chemistry The progress in this field has been very rapid even accelerating in recent years and a review appears more than justified This book offers a selection of subjects covering some of the latest developments Our primary aim is to clarify some of the basic concepts that are the most prone to misinterpretation and to provide brief introductions to some of those subjects that are expected to have further important contributions to our understanding of molecular properties and chemical reactivity **Applications of Discrete and Continuous Mathematics in Chemistry** ,1993 Publications Update World Bank,1996 Graph Polynomials Yongtang Shi,Matthias Dehmer,Xueliang Li,Ivan Gutman,2016-11-25 This book covers both theoretical and practical results for graph polynomials Graph polynomials have been developed for measuring combinatorial graph invariants and for characterizing graphs Various problems in pure and applied graph theory or discrete mathematics can be treated and solved efficiently by using graph polynomials Graph polynomials have been proven useful areas such as discrete mathematics engineering information sciences mathematical chemistry and related disciplines

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Table of Contents Discrete Mathematical Chemistry

1. Understanding the eBook Discrete Mathematical Chemistry
 - The Rise of Digital Reading Discrete Mathematical Chemistry
 - Advantages of eBooks Over Traditional Books
2. Identifying Discrete Mathematical Chemistry
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Discrete Mathematical Chemistry
 - User-Friendly Interface
4. Exploring eBook Recommendations from Discrete Mathematical Chemistry

- Personalized Recommendations
 - Discrete Mathematical Chemistry User Reviews and Ratings
 - Discrete Mathematical Chemistry and Bestseller Lists
5. Accessing Discrete Mathematical Chemistry Free and Paid eBooks
 - Discrete Mathematical Chemistry Public Domain eBooks
 - Discrete Mathematical Chemistry eBook Subscription Services
 - Discrete Mathematical Chemistry Budget-Friendly Options
 6. Navigating Discrete Mathematical Chemistry eBook Formats
 - ePub, PDF, MOBI, and More
 - Discrete Mathematical Chemistry Compatibility with Devices
 - Discrete Mathematical Chemistry Enhanced eBook Features
 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Discrete Mathematical Chemistry
 - Highlighting and Note-Taking Discrete Mathematical Chemistry
 - Interactive Elements Discrete Mathematical Chemistry
 8. Staying Engaged with Discrete Mathematical Chemistry
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Discrete Mathematical Chemistry
 9. Balancing eBooks and Physical Books Discrete Mathematical Chemistry
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Discrete Mathematical Chemistry
 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
 11. Cultivating a Reading Routine Discrete Mathematical Chemistry
 - Setting Reading Goals Discrete Mathematical Chemistry
 - Carving Out Dedicated Reading Time
 12. Sourcing Reliable Information of Discrete Mathematical Chemistry

-
- Fact-Checking eBook Content of Discrete Mathematical Chemistry
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning
- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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