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CONFERENCE ON GRAPH THEORY AND TOPOLOGY IN CHEMISTRY  
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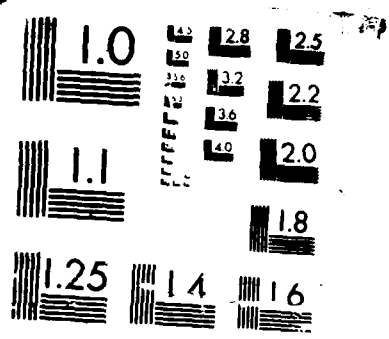
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Technical Report No. 54

Conference on Graph Theory and Topology in Chemistry

by

R.B. King and D.H. Rouvray

Prepared for Publication

in the

Proceedings of the International Conference on  
Graph Theory and Topology in Chemistry  
held in Athens, GA, March, 1987

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University of Georgia  
Department of Chemistry  
Athens, Georgia 30602

August 11, 1987

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CONFERENCE ON GRAPH THEORY AND TOPOLOGY IN CHEMISTRY

R. B. King and D. H. Rouvray, Department of Chemistry, University of Georgia, Athens

Georgia 30602

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Prof. R. B. King and Dr. D. H. Rouvray organized an International Conference on Graph Theory and Topology in Chemistry which was held at the University of Georgia, Athens, Georgia, during the period March 15-20, 1987. A volume containing the papers presented at this conference is being published by Elsevier Scientific Publishing Company, Amsterdam, and will appear around the end of 1987. The following items are attached:

- (1) The program of the conference .
- (2) The short abstracts of the paper presented at the conference .
- (3) The contents of the conference volume .
- (4) The preface of the conference volume .

→ go to p. 3 →

①

**CONFERENCE ON GRAPH THEORY  
AND TOPOLOGY IN CHEMISTRY**

**University of Georgia Center for Continuing Education  
Athens, Georgia 30602**

**March 15-20, 1987**

**Schedule of Events**

Opening Reception: Sunday, March 15, 1987

8:00 to 10:00 PM Georgia Center for Continuing Education Hospitality Suite

The Hospitality Suite will also be open on Tuesday and Thursday evenings.

A Special lunch for conference participants will be provided each day (Monday through Friday) in the Georgia Center at the times indicated in this schedule.

The Conference is scheduled to close on Friday afternoon at 12:20 PM.

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**SCHEDULE FOR MONDAY, MARCH 16, 1987**

9:00 AM            **OPENING**  
Dean W.J. Payne, College of Arts and Sciences  
University of Georgia

9:30 AM            **D.W. Sumners**  
"Knots, Macromolecules and Chemical Dynamics"

10:30 AM           **BREAK**

11:00 AM           **D.M. Walba**  
"Topological Stereochemistry: Knot Theory of Molecular  
Graphs"

12:00 PM           **D.P. Jonish and K.C. Millett**  
"Extrinsic Topological Chirality Indices of Molecular Graphs"

12:20 PM           **LUNCH**

2:00 PM            **J. Simon**  
"A Topological Approach to the Stereochemistry of Nonrigid  
Molecules"

3:00 PM            **E. Flapan**  
"Chirality of Non-Standardly Embedded Möbius Ladders"

3:20 PM            **BREAK**

3:50 PM            **M. Randić, V. Katović, D.J. Klein, W. Seitz, D.O. Oakland  
and A.T. Balaban**  
"On Symmetry Properties of Chemical Graphs: Rearrangement  
of Axially Distorted Octahedra"

7:30 PM            **Buses leave Georgia Center for Reception**

8:00 PM            **Reception at the Georgia State Botanical Garden**

10:00 PM           **Buses leave Botanical Garden for Georgia Center**

(3)



**SCHEDULE FOR TUESDAY, MARCH 17, 1987**

- 8:30 AM K. Balasubramanian  
"Computational Graph Theory"
- 9:30 AM J.R. Dias  
"Rapid Computation of the Eigenvalues of Small Heterocycles"
- 9:50 AM BREAK
- 10:20 AM D. Bonchey and O.E. Polansky  
"On the Topological Complexity of Chemical Systems"
- 11:20 AM V. Nicholson, Chun-Che Tsai, M. Johnson and M. Naim  
"A Subgraph Isomorphism Theorem for Molecular Graphs"
- 11:40 AM M. Johnson, M. Naim, V. Nicholson and Chun-Che Tsai  
"Unique Mathematical Features of the Substructure Metric Approach to Quantitative Molecular Similarity Analysis"
- 12:00 PM Chun-Che Tsai, M. Johnson, V. Nicholson and M. Naim  
"A Topological Approach to Molecular Similarity Analysis and its Application"
- 12:20 PM LUNCH
- 2:00 PM W.C. Herndon and A.J. Bruce  
"Perimeter Codes for Benzenoid Aromatic Hydrocarbons"
- 3:00 PM E.C. Kirby  
"Coding and Factorisation of Polycyclic Chemical Graphs"
- 3:20 PM S. El-Basil  
"On Data Reduction of Chemical Information"
- 3:40 PM BREAK
- 4:10 PM J.L. Bryant  
"Approximating the Total Linking Density in the Amorphous Phase of a Semicrystalline Polymer"
- 4:30 PM B. Pittel, W.A. Woyczynski and J.A. Mann Jr.  
"Random Tree-Type Partitions as a Model for Acyclic Polymerization"
- 4:50 PM R.C. Lacher  
"Measuring Entanglement in a Random Walk Model of Semicrystalline Polymer"
- 8:00 PM Informal Discussion on the International Society for Mathematical Chemistry and the new Journal of Mathematical Chemistry

**SCHEDULE FOR WEDNESDAY, MARCH 18, 1987**

- 8:30 AM O. Sinanoğlu  
"Topological Structural Covariance Method for Qualitative  
Quantum Chemical Deduction — a) Polycyclic Hydrocarbons,  
b)\* Organic Di- and Multi-Radicals"
- 9:30 AM N. Adler, K. Kovačić-Beck, N. Trinajstić  
"The Correlation Between Physical Properties and  
Topological Indices of N-Alkanes"
- 9:50 AM M.P. Hanson and D.H. Rouvray  
"The Use of Topological Indices to Estimate Melting Points  
of Organic Molecules"
- 10:10 AM BREAK
- 10:40 AM D.H. Rouvray  
"The Fractal Nature of Alkane Physicochemical Behavior"
- 11:40 AM D. Bonchey and O.E. Polansky  
"Some Relationships Between the Wiener Number and the  
Number of Self-Returning Walks in Chemical Graphs"
- 12:00 PM LUNCH
- 1:30 PM J.K. Burdett  
"Topology and the Structures of Molecules and Solids"
- 2:30 PM R.B. King  
"Topological Aspects of Infinite Metal Clusters and  
Superconductors"
- 3:30 PM BREAK
- 4:00 PM E.K. Lloyd  
"Redfield Enumeration Applied to a Chemical Problem"
- 4:20 PM B. O'Leary and R.B. Mallion  
"Counting The Spanning Trees of Labelled, Planar Molecular-  
Graphs Embedded on the Surface of a Sphere"
- 4:40 PM C. Rong-si  
"The Enumeration of Kekulé Structures of Rectangle-  
Shaped Benzenoids"
- 6:30 PM Buses leave Georgia Center for Barbecue
- 7:00 PM Barbecue at Pinecrest Lodge
- 9:30 PM Buses leave Pinecrest Lodge for Georgia Center

REVISED

SCHEDULE FOR THURSDAY, MARCH 19, 1987

- 8:30 AM D.J. Klein and S.A. Alexander  
"Organic Polyradicals, High-Spin Hydrocarbons, and Organic Ferromagnets"
- 9:30 AM L. von Szentpály  
"PMO-omega Method for Aliphatic Compounds: Bond Energies and First Ionization Energies of Alkyl Radicals and Amines"
- 9:50 AM T.P. Živković  
"Ground State Properties of Conjugated Systems in a Simple Bond Orbital Resonance Theory (BORT) Approach"
- 10:10 AM BREAK
- 10:40 AM M. Randić, S. Nikolić and N. Trinajstić  
"The Conjugated Circuits Model: On the Selection of the Parameters for Computing the Resonance Energies"
- 11:40 AM A. Graovac, D. Babić and K. Kovačević  
"The Simple Estimates of the Total and the Reference Pi-Electron Energy of Conjugated Hydrocarbons"
- 12:00 PM LUNCH
- 1:30 PM B.M. Gimarc  
"Graphs for Chemical Reaction Networks: Applications to the Isomerizations Among the Carboranes"
- 2:30 PM W.A. Seitz, D.J. Klein and T.G. Schmalz  
"Resonance and Long-Range Order in Poly-Polyphenanthrenes"
- 2:50 PM He Wenjie  
"On Kekulé Structure and P-V Path Method"
- 3:10 PM He Wenchen and He Wenjie  
"One-to-One Correspondence Between Kekulé and Sextet Patterns"
- 3:30 PM BREAK
- 4:00 PM L. Peusner  
"A Covariant Theory of Chemical Kinetic Forces based on Hill Graphs"
- 4:20 PM D.C. Mikulecky  
"Topological Contributions to the Chemistry of Living Systems"
- 4:40 PM S.B. Elk  
"A Codon Transform that Saves Storage and Eliminates Redundancy"
- 5:00 PM M.H. Lee  
"Thermodynamics of Phase Transitions in Metal Cluster Systems"

**SCHEDULE FOR FRIDAY, MARCH 20, 1987**

8:30 AM	P.G. Mezey "New Developments in Reaction Topology"
9:30 AM	L.V. Quintas "Random Graph Models for Physical Systems"
10:30 AM	CLOSING
11:30 AM	LUNCH

## KNOTS, MACROMOLECULES AND CHEMICAL DYNAMICS

D. W. Sumners

Department of Mathematics, Florida State University  
Tallahassee, Florida 32306

Knot theory is the mathematical study of placement of flexible graphs in 3-space. Configurations of macromolecules (such as polymethylene and DNA) can be analyzed (both quantitatively and qualitatively) by means of knot theory. These large molecules are very flexible, and can present themselves in 3-space in topologically interesting ways. For example, in DNA research, various enzymes (topoisomerases and recombinases) exist which, when reacted with unknotted closed circular DNA, produce enzyme-specific characteristic families of knots and catenanes. One studies these experimentally produced characteristic geometric forms in order to deduce enzyme mechanism and substrate conformation. This particular application is an interesting mix of knot theory and the statistical mechanics of molecular configurations. This paper will give a brief overview of knot theory and DNA, and will discuss a topological model for site-specific recombination.

Another interesting application of knot theory and differential topology arises in the topological description of propagating waves in excitable media. For example, in a thin layer (a 2-dimensional medium), the Belusov - Zhabotinsky reaction produces a beautiful pattern of spiral wave forms which rotate about a number of central rotor points. The waves represent points which are in phase with respect to the reaction, and the rotor points are the phaseless points--the "organizing center" of the reaction. In a 3-dimensional medium, a knot or catenane can form an organizing center for a reaction. These characteristic spiral rotating waves are seen in many biological and chemical contexts. This paper will discuss a topological model for wave patterns in 2 and 3 dimensions which relates wave patterns to a phase map. In the context of this model, a quantization condition conjectured by A.T. Winfree can be shown to be a necessary and sufficient condition for the existence of a spiral rotating wave pattern.

## TOPOLOGICAL STEREOCHEMISTRY: KNOT THEORY OF MOLECULAR GRAPHS

David M. Walba

Department of Chemistry and Biochemistry, University of Colorado

Boulder, CO 80309-0215

Chemists have always been intrigued and stimulated by consideration of the structural causes of isomerism (the phenomenon where two chemical compounds with the same number and kind of atoms exist as distinct, isolable entities). Wasserman first suggested a connection between isomerism and low dimensional topological properties of molecular graphs, and we have formalized the interface between stereochemistry and low dimensional topology by defining topological stereoisomers as molecules with molecular graphs which are homeomorphic, but not homeotopic (the term homeotopic describes graphs which are "interconvertable by continuous deformation in 3-space" and seems preferable to "isotopic" due to the lack of conflict with terms in common chemical usage). Synthesis of molecules capable of exhibiting topological stereoisomerism is one focus of our work resulting in the preparation of the first molecular Möbius strip—a 3-rung Möbius ladder with "colored" rungs. The novel topology and dynamics of the 3-rung Möbius ladder molecule will be discussed. Consideration of the topological and chemical properties of this and other topologically interesting molecules has led to the application of the techniques of knot theory to graphs. In fact, we have shown that in order to understand simple chemical properties of certain easily conceivable molecules, the techniques of low-dimensional topology must be used. The topological approach to describing molecular symmetry has also led to the discovery of an interesting new class of knots and graphs termed topological rubber gloves. These concepts will be discussed, as well as our most recent studies directed towards the synthesis of the first non-DNA trefoil knot by cutting "in half" of a 3-half twist Möbius ladder. Finally, the novel "hook and ladder" approach to the synthesis of molecular knots, which could lead to the preparation of a figure-8 knot and a topological rubber glove molecule, will be outlined.

# Extrinsic Topological Chirality Indices of Molecular Graphs

David P. Jonish and Kenneth C. Millett

Department of Mathematics, University of California  
Santa Barbara, Ca 93106

This paper presents the results of a study of the fundamental examples in an elementary class of topological stereoisomers, i.e. molecular graphs which are isomorphic graphs but whose extrinsic topological properties in 3-space distinguish between various members of the family. Specifically, we study questions of chirality (distinctness of one placement of a graph from its mirror reflection) for a family of rigid vertex 4-valent ribbon and Mobius band graphs. The different conformations are analyzed by means of the authors' chimerical graph states model which associates to each specific presentation of the graph an element of an abstract algebraic system. A brief resume of this method is given. By calculations in this associated chimerical algebra we identify algebraic indices reflecting the chiral differences between the spacial placements.

A TOPOLOGICAL APPROACH TO THE STEREOCHEMISTRY  
OF NONRIGID MOLECULES

Jonathan Simon

Department of Mathematics, University of Iowa, Iowa City, Iowa 52242

When a topologist tries to decide if two objects are "equivalent", he usually assumes everything is elastic and flexible, ignoring the very geometric details [e.g. length, angle] that are the basis of traditional stereochemistry. But there are molecular configurations (such as catenanes, knots, Mobius ladders, and others) for which topological methods may yield chemically useful information. For example, one might be able to prove that a certain highly flexible configuration is chiral, or that two of its chemically similar atoms are diastereotopic.

Our basic approach is to suppress ligands and focus on the molecular skeleton. The topological model allows unrealistic amounts of bending and stretching, but assumes the molecular graph remains intact. So when we prove that a certain pair of molecules are "topological diastereomers" that statement is chemically accurate for any range of physical conditions under which bonds cannot be made or broken. But if, say, two nuclei are "topologically homotopic", that only provides a suggestion that they might be stereochemically identical.

Our interest in topological stereochemistry is due in large part to the presentation at the 1983 Georgia symposium by D. Walba, as well as many subsequent communications with him. In this paper, we shall discuss how several of his questions have been answered and describe some mathematical tools [e.g. knot tables for graphs, topological symmetry groups] that are useful for such questions.



## CHIRALITY OF NON-STANDARDLY EMBEDDED MOBIUS LADDERS

by

Erica Flapan

### ABSTRACT

Simon has shown that the molecular mobius ladder, which was first synthesized by Walba, is topologically chiral for any  $n > 3$  rungs. That is, if  $M_n$  represents the  $n$ -rung mobius ladder as a graph, then the particular embedding of  $M_n$  in 3-space, which was synthesized by Walba, is topologically chiral. This left open the question of chirality for alternate embeddings of  $M_n$ . We show that for any  $n$  which is even there is an embedding of the  $n$ -rung mobius ladder in 3-space which is achiral, while for any  $n > 3$  which is odd every embedding of the  $n$ -rung mobius ladder in 3-space is chiral.

ON SYMMETRY PROPERTIES OF CHEMICAL GRAPHS:  
REARRANGEMENT OF AXIALLY DISTORTED OCTAHEDRA

M. Randić<sup>a</sup>, V. Katović<sup>b</sup>, D.J. Klein<sup>c</sup>, W.A. Seitz<sup>c</sup>, D.O. Oakland<sup>a</sup> and A.T. Balaban<sup>d</sup>

<sup>a</sup>Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311

<sup>b</sup>Department of Chemistry, Wright State University, Dayton, Ohio 45435

<sup>c</sup>Department of Marine Science, Texas A&M University at Galveston, Texas 77553

<sup>d</sup>Department of Organic Chemistry, Technical University, Bucharest, Roumania

We consider a rearrangement mode for axially distorted octahedra in which one of the axial ligands is exchanged for one of the equatorial ones. A single isomer then leads to eight new isomers, each of which in turn leads to new isomers. Disregarding differences among enantiomers the particular isomerization mode leads to 45 symmetry equivalent species. The isomerization graph, even though having relatively small number of vertices is nevertheless rather complex, because each of the 45 vertices has eight nearest neighbors. It is unpractical to attempt to deduce the symmetry of this graph from its pictorial representation. We outline the approach in which we use the list of neighbors and successively relabel the vertices in order to derive the canonical labels. The graph is shown to belong to symmetry group  $S_6$  (of the order 720). The search for the symmetry was manual, however it is shown how use of word-processor allows one to derive canonical labels systematically. The result adds further support to the conjecture that symmetry groups of chemical isomerization graphs are  $S_n$  (symmetric permutation group on  $n$  objects) or at most  $C_2 \times S_n$ .

## Computational Graph Theory

K. Balasubramanian\*

Department of Chemistry, Arizona State University,  
Tempe, Arizona 85207

A number of graph theoretical problems of importance in chemical applications require the use of computers. Examples of such problems are finding matching polynomials of graphs, characteristic polynomials and isomers etc. The objective of our talk would be to identify a few problems and algorithms in this new area of computational combinatorics and graph theory. The computational aspects of recursive and iterative programming techniques for finding solutions to such problems as the ones outlined above would be considered. Applications to polynomials of graphs, spectroscopy and stereochemistry would be discussed.

\* Alfred P. Sloan Fellow; Camille and Henry Dreyfus Teacher-Scholar

# RAPID COMPUTATION OF THE EIGENVALUES OF SMALL HETEROCYCLES

Jerry Ray Dias

Department of Chemistry, University of Missouri, Kansas City, MO 64110

Rapid noncomputer methods for calculating the Hückel MO characteristic polynomial and select eigenvalues of symmetrical and alternant heterocycles are presented. A functional group-like concept for recognizing the presence of select eigenvalues is detailed. The characteristic polynomial and corresponding eigenvalues of mirror plane fragments having weighted vertices belonging to over 140 different classes of symmetrical heterocycles have been computed and tabulated. These heterocycles have their heteroatoms located on the mirror plane, and their mirror plane fragments are substructural units (functional groups) that have specific eigenvalues that are present in the associated heterocycle families regardless of the identity of the heteroatom or whether there is a polyene substituent attached to these mirror plane node positions. The equations previously derived by the author are used to calculate the HMO quantities for these mirror plane fragments. Specializing one of these equations by setting  $k=0$  and  $h=-1$  leads to the following key equation  $P(G_0;X)=P(G;X)+P(G_0-V_0;X)$  where  $G_0$  is a mirror plane graph having a single weighted vertex ( $h=-1$ ),  $G$  is its isoconjugate graph, and  $G_0-V_0$  is the graph produced by deletion of the weighted vertex  $V_0$ . The concept of local symmetry will be espoused and arises within the HMO model because only 1-2 interactions are considered. Specializing the same equation by setting  $h=0$  leads to an equation useful for computing the characteristic polynomial of molecular graphs with a single weighted pendant edge.

# ON THE TOPOLOGICAL COMPLEXITY OF CHEMICAL SYSTEMS

Danail Bonchev<sup>a</sup> and Oskar E. Polansky<sup>b</sup>

<sup>a</sup>Higher School of Chemical Technology, Burgas 8010, Bulgaria

<sup>b</sup>Max-Planck-Institut für Strahlenchemie, 4330 Mülheim a.d. Ruhr,  
Federal Republic of Germany

## A B S T R A C T

The conditions are discussed which a complexity measure should meet. A general scheme for evaluating system complexity is presented which includes different hierarchical levels such as structure topology, symmetry, metrics, etc. The topological complexity is treated in detail. The structure connectedness and adjacency are regarded as essential complexity factors along with some specific features of structure topology such as branching, cyclicity, bridging, and linearity. Convenient quantitative complexity measures are introduced on this basis and some of their properties are studied.

## A SUBGRAPH ISOMORPHISM THEOREM FOR MOLECULAR GRAPHS

Victor Nicholson<sup>1</sup>, Chun-Che Tsai<sup>1</sup>, Mark Johnson<sup>2</sup>,

and Mary Naim<sup>1</sup>

<sup>1</sup>Kent State University, <sup>2</sup>The Upjohn Company

In this paper we consider the problem of identifying the maximal substructures common to two chemical structures. A subgraph isomorphism is defined by a correspondence between the vertices that preserves adjacency. Because of the enormous number of subgraphs and possible correspondences this is a formidable problem for graphs in general. A considerable reduction in the number of possibilities occurs for molecular graphs because only atoms and bonds of the same type correspond. Instead of considering correspondences between atoms, we consider correspondences between extended bonds (a bond together with its two atoms). This can produce an additional reduction by a factor of one million in the number of possible correspondences. A correspondence between extended bonds induces an isomorphism if and only if there is no interchange of triods and triangles. Since molecular graphs have few triangles the efficiency is realized in practice. The theorem has been implemented in a computer program that finds the maximal common substructures of similar compounds.

Unique Mathematical Features of the Substructure Metric  
Approach to Quantitative Molecular Similarity Analysis

Mark Johnson<sup>1</sup>, Mary Naim<sup>2</sup>, Victor Nicholson<sup>2</sup> and Chun-Che Tsai<sup>2</sup>  
<sup>1</sup>The Upjohn Company, <sup>2</sup>Kent State University

Quantitative molecular similarity analysis (QMSA) is providing new tools for searching molecular databases, selecting compounds for drug screening, predicting molecular properties and modeling drug receptor sites. A number of topological measures of molecular similarity have been proposed based on molecular fragments, topological indices and maximum common substructures. These similarity measures inherit a variety of distinguishing features from the mathematical metric spaces on which they are founded. The substructure metric is founded on a metric defined on the set of labeled graphs with multiple loops and edges. This paper reviews the unique inherited features of the substructure metric with respect to the use and analysis of molecular databases, molecular structure generation, molecular property analysis and optimization, and the incorporation of steric and electronic information into these applications.

A TOPOLOGICAL APPROACH TO MOLECULAR SIMILARITY ANALYSIS AND ITS APPLICATION

Chun-che Tsai<sup>1</sup>, Mark Johnson<sup>3</sup>, Victor Nicholson<sup>2</sup>, and Mary Naim<sup>2</sup>

<sup>1</sup>Department of Chemistry and <sup>2</sup>Department of Mathematical Sciences,  
Kent State University, Kent, Ohio 44242 and <sup>3</sup>Computational Chemistry Unit,  
The Upjohn Company, Kalamazoo, Michigan 49001

We have developed a topological approach to molecular similarity analysis for ordering, grouping, and comparing molecular structures. Several newly defined topological descriptors such as molecular topology number (NAB), maximum common substructure descriptor (MCS), molecular similarity index (MSI), molecular dissimilarity index (MDI) and topological distance descriptor (TD) have been utilized in the molecular similarity analysis. NAB denotes the number of atoms and bonds in a molecule. MCS, MSI, MDI and TD are computed, using the substructure metric, to quantify the similarity and dissimilarity between pairs of molecular structures. The substructure metric on molecular graphs defines the maximum common substructure to be the largest (sum of atoms and bonds) graph isomorphic to a subgraph in each molecular graph. The application of this topological approach to quantitative molecular similarity analysis (QMSA) and quantitative structure-activity relationship (QSAR) study will be presented.



## PERIMETER CODES FOR BENZENOID AROMATIC HYDROCARBONS

William C. Herndon and Annadora J. Bruce

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El Paso, Texas 79912

Previous coding systems for the polycyclic benzenoid aromatic hydrocarbons have generally required an optimum orientation of the molecular graph either before or during assignment of a canonical molecular code. A two-digit coding system is described in this paper that is independent of orientation and easily obtained upon examination of the perimeter of the molecular structure. An algorithm for interconversion of an adjacency matrix (connection table) and this perimeter code is presented. The use of the code to identify and locate particular types of molecular structural features is illustrated, and some applications to enumeration problems are suggested. Finally, a very simple reversible hashing procedure is described that gives rise to a useful shortened form of the code. The shortened code is shown to be identical to a unique, canonical representation of the dual inner graph of the original molecular graph.

## CODING AND FACTORISATION OF POLYCYCLIC CHEMICAL GRAPHS

E.C. Kirby

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The term factorisation is used here to mean the expression of the characteristic polynomial of a graph as a product of smaller polynomials, at least one of which corresponds to the characteristic polynomial of some other known graph. The method used is trial division, where a factor is confirmed by a division which leaves no remainder.

A number of cyclic and polycyclic structures have been examined, including in particular the set of polyhexes having 7 or fewer hexagons. About 80% of the polyhex structures examined can be factorised. Five simple tree factors were found, and these occur in 18 different combinations. The occurrence of the 2-vertex factor (corresponding to eigenvalues +1 and -1) heavily outnumbers that of any other. There exist a few apparently non-graphical polynomials which exhibit quite wide sub-spectrality; e.g. they occur as factors of a polyhex, of several trees, and of the acyclic (matching) polynomial of another cycle-containing structure. Nonbenzenoid polycyclic structures have fewer factorisable members.

The practical task of coding structural information is briefly commented upon. A code which is a good one for manipulation and recognition purposes when resident in a computer's memory, is not always as good when human input is required, and this, perhaps trivial, point seems sometimes to be forgotten or is left unstated. For example, although excellent recent work has given codes which are unique, compact, and quite easy to construct, it may still not be easy to detect errors when lists of rather similar structures have to be encoded and typed. Since at this point only accuracy of transmission without ambiguity is required (rather than uniqueness), it can be useful to interpose an intermediate code which minimises the amount of information transmitted. A useful general example is a code based on defining the ways in which a structure deviates from that of a single linear chain. For polyhexes, the use of a numbered hexagon grid provides fast encoding.

## ON DATA REDUCTION OF CHEMICAL INFORMATION

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A novel approach of data reduction and information-retrieval of many chemical graphs (of importance in chemistry and physics) is presented. Namely a bipartite caterpillar tree,  $T$ , can be associated with a nonbranched benzenoid system  $B$ , a Clar graph,  $\Lambda$ , a rook board  $P_r$  and (in certain cases) a king polyomino graph,  $P$ , such that: the characteristic polynomial of  $T$  = the sextet polynomial of  $B$  = the Clar polynomial of  $\Lambda$  = the rook polynomial of  $P_r$  = the king polyomino of  $P$ . This means that the combinatorial properties of a large graph, such as a benzenoid graph, are preserved in a much smaller graph, such as a caterpillar tree which allows that larger graphs can be studied in terms of much smaller structures. Properties studied include electronic absorption spectra, self-avoiding molecular paths, number of Kekulé structures and Sachs graphs in benzenoid hydrocarbons.

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## ABSTRACT

Approximating the total linking density in the amorphous phase of a semicrystalline polymer. John L. Bryant, Department of Mathematics, The Florida State University, Tallahassee, FL 32306

The distribution of molecules in the region between two crystal faces in a semicrystalline polymer frequently is modelled by random walk on a cubical lattice in 3-space between two planes, say  $Y=0$  and  $Y=M$  ( $M=1,2,3,\dots$ ), as proposed by DiMarzio and Guttman [*Polymer* **1980**, *21*, 733]. In his talk at this conference, Lacher explores a simplified model for estimating the expected value of the number of loops based on one plane ( $Y=M$ ) that homologically link a single loop on the other plane ( $Y=0$ ). In this talk we propose a model for approximating the density of the sum of the squares of the linking number of a loop based at  $Y=0$  with each of the loops based at  $Y=M$ . The model employs features of the simplified model together with a formula developed by Pohl [International Symposium in honor of N. H. Kuiper, Utrecht 1980, *Lecture Notes in Mathematics*, Springer-Verlag, 1981] as generalized by des Cloizeaux and Ball [*Comm. Math. Phys.* **1981**, *80*, 543]. It predicts that the total square linking density is asymptotically constant (as  $M \rightarrow \infty$ ).

**RANDOM TREE-TYPE PARTITIONS AS A  
MODEL FOR ACYCLIC POLYMERIZATION\*)**

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**ABSTRACT**

A Gaussian behavior of the subcritical sol phase and the unexpected Holtmark  $3/2$ -stable distribution of the supercritical gel are described. These results should be compared with the original Flory's model which provided just a mean value type of analysis but no information about fluctuations and with Whittle's Markov process approach where variable dissociation rates were not allowed.

- \*) Research partially supported by an SRO Grant from ONR.
- \*) Research partially done while on leave at Case Western Reserve University.

## ABSTRACT

Measuring entanglement in a random walk model of semicrystalline polymer. R.C.Lacher, Department of Computer Science, Florida State University, Tallahassee, FL 32306.

The region between two crystal faces in a semicrystalline polymer has been modelled by random walk on a cubical lattice constrained to lie in the slab between two parallel planes a distance  $M$  units apart in 3-dimensional space [Polymer 1980, 21, 733]. Loops (walks beginning and ending on the same plane) play the role of strands of polymer that exit and re-enter the same crystal while ties (walks that go from plane to opposite plane) play the role of strands that connect two crystals. A simulation has been designed to investigate the extent to which entanglement of loops may contribute to material properties. Results of the simulation indicate that two measures of entanglement (calculated from the matrix of linking numbers of a left-loop with a complete distribution of right-loops) approach positive constant values or increase without bound as  $M$  increases (while the effect of ties is known to be inversely proportional to  $M$ ) [Macromolecules, October 1986]. Simplified models, in which random loops are replaced by loops with predictable geometry, yield asymptotic estimates of some of these entanglement measures [J.Chem.Phys., November, 1986]. This talk will discuss the simulation and some of the modelling results and set the stage for the talk by Bryant on this subject.

Paper for the "Conference on Graph Theory and Topology in Chemistry"  
Athens, Georgia, March 1987

Wednesday, 8:30-9:30 a.m., March, 18, 1987

**Topological Structural Covariance Method for Qualitative  
Quantum Chemical Deductions — a) Polycyclic Hydrocarbons,  
b)\* Organic Di- and Multi-Radicals**

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ABSTRACT

a) The numbers of non-bonding (NBMO's), bonding, and anti-bonding MO's, the HOMO-LUMO types, reactivity to electro- or nucleophiles, qualitative relative stabilities of the neutral species, their anions, or cations are readily deduced for pi-polycyclics "on the blackboard" directly from the structural formulas utilizing the recently presented pictorial quantum rules. Among others, the bicyclo [p.q.0] pi-hydrocarbons are treated extensively and found to fall into ten distinct homolog classes. In addition to the customary pi-aromatic, or pi-anti-aromatic types, classes of compounds with other behaviour (e.g. one called here "anti-Kekule") are found. When an anti-aromatic ring is fused with another anti-aromatic or with a pi-aromatic ring, the resulting bicyclo-molecule is not anti-aromatic. In another series, the heptalene and other  $(4k+3)$ ,  $(4k'+3)$  bicyclics have two electrons in a single NBMO, making them "anti-Kekule". The method is able to distinguish between the properties of pairs of isomers like (s-indacene; a5-indacene) and (1,2,5,6-dibenz-pentalene; 1,2,4,5-dibenz-pentalene).

b) Organic radicals are important species as intermediates of various organic reactions. The magnetic properties of radicals with multiplicities greater than 1 may lead to significant applications. A recent qualitative quantum-chemical method was used to obtain the number of non-bonding MOs (NBMO) directly from structural formulas for organic radicals. Then the Pauli exclusion principle and Hund's rule were used to get these organic radicals' ground-state multiplicities, which were compared to experiments and other qualitative approaches and calculations. Extensive agreement was found between the present method and experiments available, as well as between the present method and other methods, which is rather encouraging.

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\*Part (b) is work done in collaboration with Mingzuo Shen of the People's Republic of China, presently at Yale University.

THE CORRELATION BETWEEN PHYSICAL PROPERTIES AND TOPOLOGICAL INDICES OF N-ALKANES

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ABSTRACT

Some physical properties of n-alkanes were examined from a structural point of view. To establish the quantitative correlation between structure and properties of n-alkanes ranging from C<sub>1</sub> to C<sub>50</sub>, the molecular descriptors which numerically represent a molecule, have been used. The suitable molecular descriptors have been chosen from the literature data on application of graph theory, and topology in chemistry.

The quantitative relations between physical properties of pure hydrocarbons and the topological indices have been checked up by the experiments with real mixture of paraffins, separated from petroleum fractions.



The Use of Topological Indices to Estimate Melting Points of Organic Molecules.

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D. H. Rouvray, Department of Chemistry, The University of Georgia, Athens, GA, 30602

ABSTRACT

Historically, topological indices have been only moderately successful in the estimation of melting points of organic compounds. In the case of linear alkanes however, the melting points can be correlated with three different topological indices with high correlation coefficients and the melting point of crystalline polyethylene is estimated within three degrees of the best estimate from thermodynamic considerations.

## THE FRACTAL NATURE OF ALKANE PHYSICOCHEMICAL BEHAVIOR

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Fractals are set-theoretic constructs that have been very extensively employed to model objects or processes which are highly irregular, fragmented, or tangled. The fractal dimension of an object, which provides a measure of the irregularity of that object, can be used to reveal unsuspected invariance characteristics or symmetries. Fractal dimensions have been found to be appropriate for the study of a wide variety of chemical objects ranging from heterogeneous surfaces to polymeric structures. Here use is made of the concept of fractal dimensionality to interpret the physicochemical behavior of normal alkane molecules. It is shown, for instance, how the fractal dimensionality accounts for the pronounced curvature seen in plots of physicochemical properties, such as the boiling point, against the carbon number. We also examine the intimate interconnection that exists between the fractal dimension and certain topological indices. A new relationship linking the exponents in Walker-type expressions to fractal dimensionalities is discussed, and a possible extension of this relationship to branched alkane species is briefly outlined.

SOME RELATIONSHIPS BETWEEN THE WIENER NUMBER AND THE NUMBER OF  
SELF-RETURNING WALKS IN CHEMICAL GRAPHS

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A B S T R A C T

Formulas are derived showing an inverse proportional dependence of the Wiener number (the half-sum of the distance matrix entries) of some special classes of graphs on the number of self-returning walks of certain length. The same type of dependence between the two graph-invariants is shown to hold also for some systematic alterations in the graph structure such as the increase in the number of branches or cycles upon the same number of vertices. In the light of the recent work of Burdett et al. the relationships found could help in understanding the various successful chemical applications of the Wiener index.

# TOPOLOGY AND THE STRUCTURES OF MOLECULES AND SOLIDS

by Jeremy K. Burdett

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Both organic and inorganic chemistry have received an enormous stimulus over the past few decades from molecular orbital theory of a simple type, namely one-electron calculations. The ideas of Fukui, Hoffmann, Hückel, Walsh and Woodward and the early work of Mulliken, which have so much moulded the way we think about the structures of molecules and their reactions, were constructed within a one-electron framework.<sup>1-5</sup> It is well known that atomic connectivity, electronegativity, and the type of orbitals carried by a particular atomic center controls to a large extent the nodal properties of the resulting molecular orbitals. Many chemical problems may be understood just by a knowledge of such orbital properties and the success of one-electron models of geometry and reactivity is in quite a large part due to this property. But what are the ingredients for this success? In this talk we will emphasise the importance of topological aspects of the electronic structure problem. We will tie together some seemingly unrelated chemical problems by showing that they have very closely related orbital solutions. We shall describe the arrangements of ligands around a central transition metal atom, the geometry of allene-like molecules, the Jahn-Teller effect in cyclobutadiene and transition metal complexes, the Peierls distortion of solids and aspects of the Woodward-Hoffman rules. The method of moments with its links to topological parameters will be a very useful way to put them on a common ground. In this way we will put the one-electron model into a wider perspective.

## TOPOLOGICAL ASPECTS OF INFINITE METAL CLUSTERS AND SUPERCONDUCTORS

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This paper summarizes the chemical bonding topology of infinite metal clusters as well as superconductors constructed from metal octahedra or metal tetrahedra. The chemical bonding topologies of discrete octahedral metal clusters can be either edge-localized (e.g.,  $\text{Mo}_6\text{X}_8\text{L}_6^{4+}$  derivatives), face-localized (e.g.,  $\text{Nb}_6\text{X}_{12}\text{L}_6^{2+}$  derivatives), or globally delocalized (e.g.,  $\text{Zr}_6(\mu_2\text{-Cl})_{12}\text{ECl}_{n-12}^{2+}$  derivatives where E = Be, B, C, N). Infinite fusion of metal octahedra in one, two, and three dimensions leads to metal cluster chains (e.g.,  $\text{Gd}_2\text{Cl}_3$ ), metal cluster sheets (e.g.,  $\text{ZrCl}$ ), and bulk metals, respectively. Superconductors exhibiting relatively high critical temperatures and magnetic fields can be constructed from edge-localized metal polyhedra such as the  $\text{Mo}_6$  octahedra in the ternary molybdenum chalcogenides (Chevrel phases) and  $\text{Rh}_4$  tetrahedra in the ternary lanthanide rhodium borides leading naturally to the concept of porous delocalization in such materials.

REDFIELD ENUMERATION APPLIED TO A CHEMICAL PROBLEM

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An old problem in chemistry is to count the number of isomers of a compound; a more recent problem is to count isomerizations. In 1981, Davidson pointed out that both problems (at least in the case of stereoisomers) may be tackled using methods of Redfield dating back to 1927. Davidson's work has been followed up by Hässelbarth and also by the present author; the latter had access to newly-available material from the Redfield family archives. In the present talk, Redfield's method will be illustrated by applying it to a chemical problem.

COUNTING THE SPANNING TREES OF LABELLED, PLANAR MOLECULAR-GRAPHS EMBEDDED ON  
THE SURFACE OF A SPHERE

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ABSTRACT

It is shown that a theorem for counting the spanning trees of labelled,  
planar, molecular-graphs, announced in 1983 by Gutman, Mallion and Essam<sup>\*</sup>,  
still applies when such graphs are embedded on the surface of a sphere.

<sup>\*</sup>I. Gutman, R. B. Mallion and J. W. Essam, Molec. Phys., 50 (1983) 859-877.

THE ENUMERATION OF KEKULÉ STRUCTURES  
OF RECTANGLE-SHAPED BENZENOIDS

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A rectangle-shaped benzenoid or simply rectangle has both "vertical" sides indented. There are two types of rectangles, i.e., prolate rectangles (with inwards indentation) and oblate rectangles (with outwards indentation). The enumeration of Kekulé structures of oblate rectangles is the topic of this paper.

The number of an oblate rectangle with  $2m-1$  tier chains of alternating lengths  $n$  and  $n+1$  is denoted by  $P_m(n)$ . It is proved that the algebraic formula for the number  $P_m(n)$  is a polynomial with factors  $(n+1)$ ,  $(n+2)^m$  and  $(n+3)$  which was conjectured by Cyvin et al. Moreover, a new fully computerized method is developed which leads to algebraic formulas for the number  $P_m(n)$ . This method is used to derive for the first time the algebraic formulas for the numbers  $P_6(n)$  and  $P_7(n)$ .



Organic Polyradicals, High-Spin Hydrocarbons,  
and Organic Ferromagnets

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The possibility of high-spin hydrocarbon species is reviewed, especially for species with conjugated  $\pi$ -networks. Several different semiempirical approaches are used to treat the lower-lying electronic states. For alternant (or bipartite) systems the predictions often take a simple qualitative form. An approach via the valence-bond model of Pauling and Wheland yields the prediction that the ground-state spin is simply half the magnitude of the difference of the number of "starred" and "unstarred" centers. At the same time this simple prediction seems to be very accurate in comparison: first, to complete configuration-interaction calculations on Parisier-Parr-Pople models; second, to accurate brute-force ab initio computations; and third, to experiment. In addition, to purely  $\pi$ -network hydrocarbon polyradicals, extensions to other species are made, including: aromatic carbenes, some hetero-atom species, and to intermolecular exchange coupling as in crystals. In the latter circumstance with a suitable arrangement of molecules, predictions for the occurrence of organic ferromagnets arise.

*Quantum Chemical* STRUCTURE-REACTIVITY RELATIONSHIPS IN  
POLYCYCLIC BENZENOID AROMATIC HYDROCARBONS

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Abstract: Theoretical methods to predict chemical reactivity properties of polycyclic benzenoid aromatic hydrocarbons (PBAH) are reviewed. These methods include the usual molecular orbital quantum chemical calculations, and also pencil and paper MO and valence bond procedures to derive indices related to the rates of chemical reactions. Justification for the pencil and paper procedure termed PMO:F (Perturbational Molecular Orbital:Free Electron Method) is presented, and the modifications (PMO:F $\omega$ ) of this procedure necessary to handle the differing reactivity patterns with neutral and ionic intermediates are also given. Examples of correlations of experimental results are used to illustrate these modifications.

GROUND STATE PROPERTIES OF CONJUGATED SYSTEMS IN A SIMPLE BOND ORBITAL  
RESONANCE THEORY (BORT) APPROACH<sup>a</sup>

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ABSTRACT

A simple BORT approach is used in order to analyze ground state properties of conjugated systems. In the case of alternant hydrocarbons, ground state  $\Psi$  contains only these BORT Kekulé structures which have the same parity. In addition, all these structures are contained in  $\Psi$  with the same sign. Neglecting excited BORT structures, this implies a set of qualitative relations concerning bond orders in the ground state. Using the ansatz that all these BORT Kekulé structures contribute equally to the ground state, approximate quantitative expressions for the ground state energies and bond orders are derived. Nonalternant systems and conjugated systems containing heteroatoms are treated as perturbed alternant systems. A set of qualitative and approximate quantitative relations is obtained for such systems. In particular, simple rules concerning effective charges, bond orders and polarisabilities are obtained. Some of these rules coincide with the rules derived independently within the MO approach in the simple Hückel approximation, and some are new. Using these rules and the corresponding quantitative relations, one can predict in a simple way and without any extensive calculation many ground state properties of conjugated systems. Qualitative prediction is quite reliable, but the quantitative is less so, since it is subject to various errors due to the approximate nature of the above treatment.

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<sup>a</sup>Research supported by the Robert A. Welch Foundation of Houston, Texas.

THE CONJUGATED CIRCUITS MODEL: ON THE SELECTION OF THE  
PARAMETERS FOR COMPUTING THE RESONANCE ENERGIES

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The conjugated circuits model (ref. a) is revisited. A novel set of parameters for the resonance energy calculations within the framework of the conjugated circuits model is proposed. Resonance energies obtained with these parameters are compared to those calculated by Randić's original parameters (refs. a,b) and by Herndon's parameters (ref. c). Besides conjugated hydrocarbons, some heterocyclic systems containing either a single (pyridine-like or pyrrole-like) nitrogen atom, or a single (furan-like) oxygen atom or a single (thiophene-like) sulphur atom are also considered.

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- b. M. Randić, J. Am. Chem. Soc. 99, 444 (1977).
- c. W.C. Herndon, Israel J. Chem. 20, 270 (1980).

THE SIMPLE ESTIMATES OF THE TOTAL AND THE REFERENCE PI-ELECTRON  
ENERGY OF CONJUGATED HYDROCARBONS

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Simple purely non-empirical formulae for the evaluation of the Hückel and the reference pi-electron energies are derived. These approximative formulae contain only simple topological invariants of the appropriate molecular graphs. Although the correlation between exact and approximative values is very good, it is not sufficient to enable a reliable estimation of the topological resonance energy, TRE.

GRAPHS FOR CHEMICAL REACTION NETWORKS:  
APPLICATIONS TO THE ISOMERIZATIONS AMONG THE CARBORANES

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The representation of chemical reaction networks as graphs, with reactant and product structures as graph vertices and reaction processes as graph edges, is hardly a novel idea. Such graphs have been prepared to describe metabolic reactions, organic synthesis trees, and permutational isomerizations observed in fluxional molecules. Graphs that map the interconversions of positional isomers provide particularly simple but practical examples. These isomerizations produce new molecules with different energies but maintain the same structural framework. No additional reactant species are required and no fragment products are discarded along the way. Processes that permute otherwise identical atoms may be omitted. Reaction network graphs related to specific mechanistic proposals can be combined with calculated total energies of the various isomers and with experimental observations to assess the validity of proposed mechanisms.

In this paper, reaction network graphs will be presented for isomeric rearrangements of the closo-carboranes,  $C_2B_{n-2}H_n$ ,  $n = 5$  through 12. In these molecules, carbon and boron atoms form closed polyhedral cages with triangular faces and exo-substituted hydrogens. The location of the pair of carbon heteroatoms in the polyhedral framework introduces the possibility of two or more positional isomers for each carborane. Processes that have been proposed for these isomerizations include the diamond-square-diamond mechanism, the triangular face rotation mechanism, and the single edge cleavage process. Network graphs for these rearrangements will be discussed in relation to ab initio SCF MO calculated energies of individual isomers and a summary of pertinent experimental observations.

"Resonance and Long-Range Order in Poly-Polyphenanthrenes"

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Abstract

Herndon-Simpson quantitative resonance theory or equivalently Randic's conjugated circuit method is applied to poly-polyphenanthrene polymers. Ground state energy estimates are obtained for increasingly wide polymer strips with extrapolation to the energy of the graphite lattice. Results are compared to valence-bond theory within the resonance theoretic approximation, Clar-type structure energy estimates and Kekulé count evaluations. The calculation employs a generalization of the transfer matrix Kekulé count method applied previously to these systems. Long-range spin-pairing order is noted to occur with consequent bond localization. Solitonic excited states can occur in which an exciton separates different (but energetically near-degenerate) spin-pairing phases.

## ON KEKULÉ STRUCTURE AND P-V PATH METHOD

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### Abstract

In this paper, a new constructive method, P-V path method, is developed, which allows easily to distinguish whether there exists any Kekulé structure for an HF-graph (a honeycomb fragment graph) and to construct its one of Kekulé structures. Based on some properties of P-V paths, the relation between P-V path method and the max-flow min-cut theorem in the network theory is proposed. Using the max-flow min-cut theorem, we obtain some other theorems about the existence of the Kekulé structures.



# ONE-TO-ONE CORRESPONDENCE BETWEEN KEKULÉ AND SEXTET PATTERNS

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Ohkami-Hosoya conjecture is a well known conjecture of CAS(Clar aromatic sextet) theory:

For any benzenoid hydrocarbon(polyhex graph), which has at least one Kekulé pattern, there exists a one-to-one correspondence between Kekulé and sextet patterns.

In this paper, we investigate the conjugated circuit structure of KHF systems and give the proof of the Ohkami-Hosoya conjecture.

So called a KHF graph is a planar honeycomb fragment graph which has at least one Kekule pattern, i.e. it has at least one composition into 1-factors.

At first we prove that in any Kekulé pattern of a KHF graph without vertices of degree one, there exists at least one basic circuit which is a conjugated circuit.

Then we prove that for any KHF graph G(without vertices of degree one), there is one and only one Kekulé pattern in which all the conjugated circuits are right(left).

After that we give the definition of a super sextet.

Finally, we prove that for any given orientation of any KHF graph, there exists a one-to-one correspondence between Kekulé and sextet patterns. Specifically, in the case of benzenoid hydrocarbons, this proof becomes the proof of the Ohkami-Hosoya conjecture.

**ABSTRACT. A Covariant Theory of Chemical Kinetic Forces based on Hill Graphs.**  
Leonardo Peusner, L.P.A. Inc, Portland, Maine 04101.

A theory of Kinetic Forces is presented in which the resultant forces are properly conjugate to the kinetic rates, in analogy with the thermodynamic situation. A non-linear reversibilization of the well known Hill/King-Alman graphs yields the desired forces for a restricted family of transition processes. The resultant (covariant) theory provides a dissipation like kinetic function and is invariant under transformations of reference levels. The relationship to D'Alembert's principle, Lagrangian formulations and limited reciprocities are studied. Application examples include: linear, branched and loop reactions, convection, reaction diffusion transport and radiation.

TOPOLOGICAL CONTRIBUTIONS TO THE CHEMISTRY OF LIVING SYSTEMS

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This paper illustrates some applications of Peusner's Network Thermodynamics (L. Peusner, Studies in Network Thermodynamics, Elsevier, 1986) to the study of the physical chemistry of living systems. It focuses on some general notions which were the building blocks of Rashevsky's "Relational Biology" first spelled out in his 1954 paper entitled "Topology and Life" (Bull. Math. Biophys. 16:317-348, 1954.) Relational Biology has recently been given further attention by Rosen (Theoretical Biology and Complexity, Academic Press, 1985). Rosen distinguishes between complex systems and simple systems or mechanisms on the basis of the kinds of information needed to explain them. His criteria suggest that there is a congruence between Rashevsky's original assertion that mathematical biology needed to pay more attention to topological characteristics of living systems to balance the emphasis on what he termed the "metric" aspects and Peusner's demonstration that network thermodynamics relates a system's topology to its geometry in a clear, systematic way. These ideas are illustrated in a simple example of epithelial transport to show that the explanation of an important phenomenon in certain epithelial membranes is largely found in the topology of the system, in spite of the fact that it has a very simple topology. Furthermore, it will be shown that the same topological properties exist in an adjacent portion of the membrane and suggest that the now classical explanation needs to be augmented by a second, intrinsically equivalent mechanism working in harmony with it.

A CODON TRANSFORM THAT SAVES STORAGE AND ELIMINATES REDUNDANCY

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ABSTRACT

Using the principles inherent in the efficient storage of information in a computer assembly language, an analogous explanation of the number of amino acids present in the genetic code is given. This explanation is based on cryptographic and informational science models using a variable, instead of the more familiar fixed, length codon system. It is, therefore, suggested that, perhaps in the early development of life, a one-to-one onto relation between t-RNA and the 20 amino acids was present. Note that, through the elimination of redundancy, the proposed codon system would result in a saving of from 16 2/3% to 50% in the amount of information that had to be transmitted.

# THERMODYNAMICS OF PHASE TRANSITIONS IN METAL CLUSTER SYSTEMS\*

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Metal clusters are finite- $N$  body systems, which may be regarded as precursors to an infinite many-body structure. The statistical thermodynamics of these finite systems has been approached by placing these clusters on a lattice. Within mean field theory one can calculate thermodynamic properties by considering certain "most singular" lattice diagrams, which are also summable. Recent developments show that mean field treatments can be further extended by a  $1/N$  expansion technique, where  $N$  is the number of particles in a cluster. This new analytic technique provides an attractive way to study incipient phase transitions such as the metal-insulator transition, resulting from the growth of  $N$ .

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## NEW DEVELOPMENTS IN REACTION TOPOLOGY

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Chemical reactions can be represented by topological relations on potential energy hypersurfaces. These relations are of importance in computer-based synthesis design and molecular engineering. The properties of the reduced nuclear configuration space, metric space  $M$ , allow for a concise representation of such chemical processes. This  $(3n - 6)$ -dimensional space  $M$  has some counterintuitive properties, for example, some reaction paths show "reflections" at certain internal nuclear configurations. In this study a fundamental property of space  $M$  is demonstrated that is a condition for coordinate systems and differentiability on  $M$ . Set  $M$  can be converted into a manifold with boundary.

## RANDOM GRAPH MODELS FOR PHYSICAL SYSTEMS

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Loosely speaking a "random graph" means a graph generated by some random process. This process can be either the result of some natural physical phenomenon such as polymerization or percolation, both of which have been studied via graph theory, or the process can be the result of a man-made action such as a computer simulation or some other non-computerized random device. A third type of graph is one obtained by purely mathematical assumptions.

It is clear that in each of the above three classes the graphs to be studied have to be precisely defined in order to carry out computations and to be able to interpret the results. In particular, if theoretical or simulation models are to be applied to physical systems one must be extremely careful in describing the model being used so that anyone applying the results will be able to verify if they indeed apply to their specific situation.

We shall discuss probability models for graphs having no point of degree greater than some fixed number  $f$ . Such graphs are called  $f$ -graphs and in this context are called random  $f$ -graphs. We shall then discuss a computer simulation program for these random  $f$ -graphs and conclude with remarks concerning the pros and cons of the physical applications of these models.

## CONTENTS

### Preface

### List of Authors

#### Section A: Knot Theory and Reaction Topology

1

Knots, Macromolecules and Chemical Dynamics  
D.W. Sumners

Topological Stereochemistry: Knot Theory of Molecular Graphs  
D.M. Walba

A Topological Approach to the Stereochemistry of Nonrigid Molecules  
J. Simon

Chirality of Non-Standardly Embedded Möbius Ladders  
E. Flapan

Extrinsic Topological Chirality Indices of Molecular Graphs  
D.P. Jonish and K.C. Millett

New Developments in Reaction Theory  
P.G. Mezey

An Outline for a Covariant Theory of Conservative Kinetic Forces  
L. Peusner

Topological Contributions to the Chemistry of Living Systems  
D.C. Mikulecky

#### Section B: Molecular Complexity, System Similarity, and Topological Indices

On the Topological Complexity of Chemical Systems  
D. Bonchev and O.E. Polansky

Numerical Modelling of Chemical Structures: Local Graph Invariants  
and Topological Indices  
A.T. Balaban

The Fractal Nature of Alkane Physicochemical Behavior  
D.H. Rouvray

The Correlation between Physical Properties and Topological Indices  
of N-Alkanes  
N. Adler and L. Kovačič-Beck

The Use of Topological Indices to Estimate the Melting Points of  
Organic Molecules  
M.P. Hanson and D.H. Rouvray

Some Relationships between the Wiener Number and the Number of Self  
Returning Walks in Chemical Graphs  
D. Bonchev, O. Mekenyan and O.E. Polansky



Unique Mathematical Features of the Substructure Metric Approach to Quantitative Molecular Similarity Analysis M. Johnson, M. Naim, V. Nicholson and C.-C. Tsai	21
A Subgraph Isomorphism Theorem for Molecular Graphs V. Nicholson, C.-C. Tsai, M. Johnson and M. Naim	21
A Topological Approach to Molecular-Similarity Analysis and its Application C.-C. Tsai, M. Johnson, V. Nicholson and M. Naim	21
<b>Section C: Polyhedra, Clusters and the Solid State</b>	23
Permutational Description of the Dynamics of Octacoordinate Polyhedra J. Brocas	23
Symmetry Properties of Chemical Graphs X. Rearrangement of Axially Distorted Octahedra M. Randic, D.J. Klein, V. Katovic, D.O. Oakland, W.A. Seitz and A.T. Balaban	26
Graphs for Chemical Reaction Networks: Applications to the Isomerizations Among the Carboranes B.M. Gimarc and J.J. Ott	29
Topology and the Structures of Molecules and Solids J.K. Burdett	30
Topological Aspects of Infinite Metal Clusters and Superconductors R.B. King	32
Thermodynamics of Phase Transitions in Metal Cluster Systems M.H. Lee	34
Random Graph Models for Physical Systems K.T. Balinska and L.V. Quintas	34
From Gaussian Subcritical to Holtzmark ( $3/2$ - Levy Stable) Supercritical Asymptotic Behavior in "Rings Forbidden" Flory-Stockmayer Model of Polymerization B. Pittel, W.A. Woyczynski and J.A. Mann	36
<b>Section D: Eigenvalues, Conjugated Systems, and Resonance</b>	37
Ground-State Multiplicities of Organic Di- and Multi-Radicals M. Shen and O. Sinanoglu	37
Organic Polyradicals, High-Spin Hydrocarbons, and Organic Ferromagnets D.J. Klein and S.A. Alexander	40
Ground State Properties of Conjugated Systems in a Simple Bond Orbital Resonance Theory (BORT) T.P. Živkovic	42
The Conjugated Circuits Model: On the Selection of the Parameters for Computing the Resonance Energies M. Randic, S. Nikolic, and N. Trinajstić	42
Simple Estimates of the Total and the References Pi-Electron Energy of Conjugated Hydrocarbons A. Graovac, D. Babić, and K. Kovačević	44

Resonance in Poly-Polyphenanthrenes: A Transfer Matrix Approach W.A. Seitz, G.E. Hite, T.G. Schmalz and D.J. Klein	47
Rapid Computation of the Eigenvalues of Small Heterocycles using a Functional Group-like Concept J.R. Dias	47
On Kekule Structure and P-V Path Method H. Wenjie and H. Wenchen	47
One-to-One Correspondence between Kekule and Sextet Patterns H. Wenchen and H. Wenjie	48
<b>Section E: Coding, Enumeration and Data Reduction</b>	48
Perimeter Codes for Benzenoid Aromatic Hydrocarbons W.C. Herndon and A.J. Bruce	48
Computational Graph Theory K. Balasubramanian	50
Coding and Factorisation of Polycyclic Chemical Graphs E.C. Kirby	50
Redfield Enumeration Applied to Chemical Problems E.K. Lloyd	50
Counting the Spanning Trees of Labelled, Planar Molecular Graphs Embedded on the Surface of a Sphere B. O'Leary and R.B. Mallion	54
The Enumeration of Kekule Structures of Rectangle-Shaped Benzenoids C. Rong-si	55
Graphs of Chemistry and Physics: On Data Reduction of Chemical Information S. El-Basil	55
Index	57

## PREFACE

The burgeoning growth of chemical graph theory and related areas in recent years has generated the need for increasingly frequent conferences covering the area of mathematical chemistry. This book contains the papers presented at the International Conference on Graph Theory and Topology in Chemistry held at the University of Georgia, Athens, Georgia, U.S.A., during the period March 15-20, 1987. This Conference was in many ways a sequel to a symposium held at our university in April, 1983, the papers from which were also published by Elsevier in a special symposium volume. Both of these meetings were sponsored by the U.S. Office of Naval Research.

The principal goal of our Conference was to provide a forum for chemists and mathematicians to interact together and to become better informed on current activities and new developments in the broad areas of chemical topology and chemical graph theory. The purpose of this book is to make available to a wider audience a permanent record of the papers presented at the Conference. The 41 papers contained herein span a wide range of topics, and for the convenience of the reader have been grouped into five major sections. Although we appreciate that any such subdivision of the Conference presentations will always be somewhat arbitrary, we hope that grouping the papers in this way will help the reader to locate those papers of particular personal interest with greater facility.

Our Conference also provided an ideal setting for launching the newly established Journal of Mathematical Chemistry, edited by Dr. D.H. Rouvray. A complimentary copy of the first issue of this journal was distributed to every Conference participant. As participants came from ten different countries, namely Bulgaria, Canada, China (People's Republic), Egypt, Great Britain, India, Japan, Mexico, the United States, and Yugoslavia, a wide circulation of the new journal was assured. During the Conference the fledgling International Society for Mathematical Chemistry was also discussed and several decisions taken. Thus, in addition to purely scientific matters, a number of other issues were addressed by our Conference.

The Conference could not have been the success it was without the support of a number of organizations and individuals whom we should like to thank publicly here. We are indebted to the U.S. Office of Naval Research for the major financial support that made our Conference possible. Local support from the University of Georgia

Research Foundation and the University of Georgia School of Chemical Sciences is also acknowledged. Mention must also be made of the sterling efforts of Mr. David Payne of the Georgia Center for Continuing Education in coordinating arrangements for the Conference, and of the quiet efficiency of our secretary, Ms. Ann Lowe, who kept track of numerous administrative details and who assisted greatly in the production of this Conference volume.

University of Georgia  
Athens, Georgia  
June, 1987

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-8