

# Topological Approach To The Chemistry Of Conjugated Molecules

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## **Graph theoretical approach to the topological spin**

January 9th, 2019 - Volume 134 number 6 CHEMICAL PHYSICS LETTERS 20 March 1987 GRAPH THEORETICAL APPROACH TO THE TOPOLOGICAL SPIN HAMILTONIAN APPLIED TO CONJUGATED MOLECULES J CIOSLOWSKI Department of Chemistry Georgetown University Washington DC 20057 USA Received 31 October 1986 in final form 15 December 1986 Approximate formulae for the total  $n$  electron energy calculated within the topological spin Hamiltonian are derived using the connected moments expansion CMX technique up to the third order

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January 4th, 2019 - The topological approach to chemistry in general and

to conjugated structures in particular has flourished in the last decade for several reasons

### **A substructure based topological quantum chemistry**

January 7th, 2019 - The linear conjugated compounds are a class of important organic compounds with good ultraviolet UV absorption which are usually employed as the parent molecules of a lot of optical materials The traditional topological quantum chemistry approach can accurately predict the UV absorption energies of unsubstituted linear conjugated alkenes

### **Ante Graovac and Chemical Graph Theory**

January 11th, 2019 - or "topological" approach to conjugated molecules was a volume in the Springer Lecture Notes Series co authored by Graovac Gutman and Trinajstić 1 In the seventies and early eighties his favourite graphs were benzenoids and other planar molecular graphs arising from hydrocarbons

### **Topological Studies on Heteroconjugated Molecules A New**

January 9th, 2019 - Topological Studies on Heteroconjugated Molecules A New Pairing Theorem Topological approach to the chemistry of conjugated molecules Graphs Representing Conjugated Molecules 2 3 1

### **Topological studies on heteroconjugated molecules Springer**

December 7th, 2018 - Preliminary topological results on alternant molecules with one heteroatom were reported in 3 The way in which a heteroconjugated molecule is represented by a graph is described in detail elsewhere 3 4 For example G and Gg are the molecular graphs of acridine I and diphenylamine II respectively

### **00 A GRAPH THEORETICAL AND TOPOLOGICAL APPROACH**

January 12th, 2019 - A Graph Theoretical and Topological Approach to Final Report May 15 1984 Chemical Structure Reactivity and Dynamics to September 30 1988 Chemistry has been responsible for the overall direction of this group and for the BnHn2 and related molecules for comparison with the predictions from graph theoretical and topological methods

### **Mathematical chemistry Wikipedia**

January 11th, 2019 - Mathematical chemistry is the area of research engaged in novel applications of mathematics to chemistry it concerns itself principally with the mathematical modeling of chemical phenomena Mathematical chemistry has also sometimes been called computer chemistry but should not be confused with computational chemistry

### **I Gotman Books List of books by author I Gotman**

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### **Exciton Scattering on Symmetric Branching Centers in**

January 9th, 2019 - in Conjugated Molecules ABSTRACT The capability of the exciton scattering approach an efficient methodology for excited states in branched conjugated molecules is extended to include symmetric triple and chemistry We introduce topological charges associated with

## A novel topological index for coding of alternant systems

December 9th, 2018 - 16 Groavac A Gutman I amp Trinajstic N Topological approach to the chemistry of conjugated molecules Springer Verlag Berlin 1977 17 Gutman I amp Polansky E Mathematical concepts in organic chemistry Springer Verlag Berlin 1977 18 Proskuryakov IV Problems in algebra Mil Publishers Moscow 1978

## Topology chemistry Wikipedia

January 7th, 2019 - Molecular topology is a part of mathematical chemistry dealing with the algebraic description of chemical compounds so allowing a unique and easy characterization of them Topology is insensitive to the details of a scalar field and can often be determined using simplified calculations

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