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334 J. Chem. InJ Comput. Sci. 1985, 25, 334-343 Applications of Graph Theory in Chemistry ALEXANDRU T. BALABAN Department of Organic Chemistry, Polytehnice Institute. 76206 Bucharest, Roumania Received March 12. 1985 Graph theoretical (GT) applications in chemistry underwent a dramatic revival lately. Con-

### **334 J. Chem. InJ Comput. Sci. 25, 334-343 Applications of**

Sunil Jayant Kulkarni. Graph Theory: Applications to Chemical Engineering and Chemistry Galore International Journal of Applied Sciences and Humanities (www.gkpublication.in) 18

### **Graph Theory: Applications to Chemical Engineering and**

Application of Chemical Graph Theory for Automated Mechanism Generation Artur Ratkiewicz\*,<sup>1</sup> and Thanh N. Truong\*,<sup>2</sup> Henry Eyring Center for Theoretical Chemistry, Department of Chemistry, University of Utah, 315 South

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For example, finding a transversal, i.e., the problem of obtaining a zero-free diagonal of a sparse matrix after permuting its rows and columns, can be solved via bipartite matching algorithms [12].

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Applications of graph theory in chemistry. Alexandru T. Balaban. J. Chem. Inf. Comput. Sci., ... Application of Chemical Graph Theory for Automated Mechanism Generation. Artur Ratkiewicz and Thanh N. Truong. ... Chemical applications of graph theory. Part I. Fundamentals and topological indices

### **Applications of graph theory in chemistry - Journal of**

tered on chemical applications of graph theory including an overview of the interactions between chemistry and discrete mathematics. A few previous ... Chemical Graph Theory and the Sherlock Holmes Principle 109 Table 1. Equivalence between chemical and mathematical terms

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Chemical Applications of Graph Spectral Theory In this bibliography are included books and expository articles that are either completely or to a significant extent concerned with some aspect(s) ...

### **(PDF) Chemical Applications of Graph Spectral Theory**

Chemical graph theory (CGT) is a branch of mathematical chemistry which deals with the nontrivial applications of graph theory to solve molecular problems. In general,

### **Chemical Graph Theory - Estrada Lab**

The field graph theory started its journey from the problem of Königsberg bridge in 1735. This paper gives an overview of the applications of graph theory in heterogeneous fields to some extent but mainly focuses on the computer science applications that uses graph theoretical concepts.

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