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Entropy bounds for hierarchical molecular networks

Analysis Applications of Hierarchical Graphs. In this section, we briefly outline some applications of hierarchical graphs in chemical graph theory and computational

Graph theory in chemistry and drug design - crc

Features; Includes special chapters that address the computational aspects of chemical graph applications; Presents chemical graphs and graph algorithms with examples

Molecular graph theory applied to fullerenes

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Introduction to graph theory - springer

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Handbook of applied algorithms:solving scientific

The field of chemical graph theory utilizes simple graphs as models of molecules. These models are called molecular graphs, and quantifiers of molecular graphs are

Information-theoretic methods in chemical graph

Information-Theoretic Methods in Chemical Graph Theory Elena D.H. (ed.) Computational Chemical Graph Theory. Nova Science Publishers, New York (1990)

Research group - chemistry

Development and application of theoretical and computational methods for studying structure, reactivity, spectroscopy of chemical processes in different environments.

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Math danail bonchev

Graph theory, network theory, Section Editor for Complexity in Computational Chemistry, Encyclopedia of Complexity and Systems Science, Springer, New York.

Fourth generation detour matrix-based topological

has keen interest in computational chemistry and in-silico drug discovery. In the chemical graph theory, chemical structures are simply represented as hydrogen

Computational chemical graph theory, dennis h

Computational chemical graph theory, Dennis H. Rouvray, ed., Nova Science Publisher, Inc., New York, 1990, 331 pp. ISBN 1-947143-84-5. Price: \$72.00

Transition state theory - university of michigan

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