



2012 HAWAII UNIVERSITY INTERNATIONAL CONFERENCES
EDUCATION, MATH & ENGINEERING TECHNOLOGY
JULY 31ST TO AUGUST 2ND
WAIKIKI BEACH MARRIOTT RESORT & SPA
HONOLULU, HAWAII

APPLICATIONS OF TREE EXPRESSIONS
FOR ATOM AND BOND
IDENTIFICATION
DISCRETE MATHEMATICS/LINEAR
ALGEBRA WITH APPLICATIONS IN
CHEMISTRY

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Applications of Tree Expressions for Atom and Bond Identification

Discrete mathematics/linear algebra with applications in chemistry

Tree expressions generalize continued fractions. We motivate the definition of a tree expression and provide a connection between tree expressions and quotients of determinants of specialized matrices. Finally, we demonstrate two applications of tree expressions for classifying atoms and bonds in chemical compounds by their local environments.

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Abstract

Tree expressions generalize continued fractions; a continued fraction is a tree expression where the tree in question is a path. In turn, the numerical value of a tree expression can be determined as the quotient of two determinants which facilitates a further generalization to graphs that contain cycles. We demonstrate two applications of such computations to classifying local chemical structures. The first uses the determinant quotient to categorize atoms by their local neighborhood structure whereas the second uses tree expressions directly to categorize bonds by their local structure. Such expressions form the basis for quick identification and classification schemes of local structures for chemical compound analysis and high-throughput drug design.