Chemical Applications of Graph Theory

Readers of the *Journal of Chemical Information and Computer Sciences* during the last year or two will have noticed the increasing number of papers on chemical graph theory. In 1991, over 20% of the papers in *JCICS* were in this area, making it the leading area of interest for our authors. Graph theory is an important and exciting area of computer science and chemistry, and the content of *JCICS* reflects this. This current issue contains 10 papers that were presented at a symposium on graph theory held during the fall ACS meeting in New York City, and in addition, two other papers on the subject are included.

Treating chemical structures as graphs whose vertices are atoms and edges are bonds is becoming an important new methodology in chemistry because such graphs permit an understanding of structure and reactivity. The study of the mathematical characteristics of chemical structures is valuable because structure–property relationships derived exclusively from these mathematical characteristics hold for all related structures. Discrete mathematics, the study of finite systems, includes vectors, matrices, set theory, graph theory, combinatorics, and relations. Mathematical theories can stand alone, but chemical theories must satisfy both chemical and mathematical logic. Translation of chemical data into mathematical descriptions is achieved by creation of the appropriate connecting framework and chemical graph theory is an example of such a framework.

Chemical graph theory is valuable in studies of the *relationships* defined by the pattern of interatomic bonds in a molecule. A molecular structure can be characterized reproducibly and unambiguously as a mathematical expression derived from *graphical invariants*, so named because they reflect only the connectivity of the molecule, not the way in which it is oriented or in which its atoms are numbered. This fact underlies most modern structure and substructure search algorithms. The mathematical expression has no chemical content and to connect it firmly to the chemistry of the associated molecule, it is necessary to provide measured numeric data for selected standard molecules. In this way, the chosen graph-theoretical parameters are calibrated, and if the model is adequate, they will allow the prediction of the same properties for other structures. Numerous relationships between such mathematical expressions and the physical and chemical properties of the structure are now known and more are reported every month.

This approach is used in a number of the papers in this issue. Klein's group shows that relationships exist between chemical graphs and the magnetic susceptibilities of the molecules they represent, Herndon and Garbalena report that the enthalpies of alkanes can be calculated from the appropriate chemical graphs, and Schultz et al. show that the boiling points of alkanes can similarly be predicted. Graph theory greatly facilitates problems of isomer enumeration, and papers by Dias and by Cyvin illustrate how this can be exploited in studies of aromatic systems. Graph-theoretical enumeration methods are applied by Balasubramanian to gallium arsenide clusters as well as buckminsterfulleranes, and Elk proposes rules for the nomenclature of the isomeric regular polyhedranes. King applies graph theory to a study of aromaticity in inorganic compounds, and Hall shows how a similar approach can be used to compute the distribution of eigenvalues, or energy levels, in alternant hydrocarbons. Finally, the fertile area of topological indices—mathematical functions derived from structures—is revisited by Trinajstić, who reviews the major indices that are known; by Randić, who examines the potential of graphs in the determination of molecular similarity; and by Balaban, who reports third-generation topological indices which carry information concerning heteroatoms and bond types.

Almost all the players in the world contributed to this symposium, and the papers in this issue offer a useful perspective on this *nexus* of mathematics and chemistry. Some gifted people have been attracted to chemical graph theory and have developed it into a discipline which should be watched by anyone interested in computer manipulation of chemical structures.

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