

Review of *Applied Finite Group Actions* by A. Kerber (Springer, Berlin, 1999)

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This book provides a comprehensive treatment of the combinatorial theory associated with the classification, generation, and enumeration of a variety of discrete mathematical structures, with the classification mediated by a group action on the structures. Such structures notably include molecular graphs, geometrical embedding classes of graphs, molecular reactions, quantum symmetry-adapted states, and a variety of other (chemical, physical, or mathematical) graphical and combinatorial species of interest. And the group actions involve not only point-group symmetries of 3-dimensional structures, but also especially permutational symmetries, e.g., connected with the different ways of arranging a ligand or functional group in a molecule. The idea of enumeration of structural (or constitutional) isomers is but one historically important aspect of the currently developed theory. And the ideas apply to different types of isomer classification, and even different types of groupings of related isomers. Kerber's development seeks to adhere to a maximum of generality, often encompassing what have otherwise been viewed as different approaches to the same material, and further, mathematical proofs occur throughout. Thence a formidable amount of nomenclature and notation is used, and much perseverance is required of a typical chemical reader. In this regard, chapter 11 surveying some background material is useful, and in as much as symbols once defined are oft repeatedly used long afterwards without redefinition, the (long) list of symbols (following the table of contents) is very useful. But the rewards of perseverance seem promising in the generality attained, presumably with many new chemical applications possible. The book focuses on the correspondence between various structures and mathematical mappings, so as to facilitate going much beyond classical enumeration. Subclassifications perhaps with a requirement or preclusion of different substructures are considered, and the generation of structures (as identified by their combinatoric correspondents) is also an aspect considered. Explicit attention is in fact paid to chemistry, as one might suspect from the molecular structural formula for dioxin appearing on the outside back cover of the book. Chemical applications appear in several points in the text, including: some parts of section 2.1, all of section 3.4 (entitled "Chemical Applications"), some parts of section 7.1 (where combinatorial chemical libraries make an appearance), some parts of section 9.4, and a surprising amount of the section 12.1 (on the history of the subject of the book).

Though the bulk of the book is quite mathematical, it really offers insight to the interconnection between mathematical developments and chemical problems. The easily read section 12.1 provides a modicum of history of chemical-enumeration methodology oft foregone in standard histories of chemistry, or of mathematics. Fundamental mathematics by A. Cayley and particularly by G. Pólya were in fact motivated from chemistry, to which these authors also made seminal contributions. More recent developments by N.G. deBruijn, by R.C. Read, by E. Ruch, and by A. Kerber, as well as members of his group, have also had chemistry as at least a partial motivation. Thence in addition to the primary focus on the combinatorial equivalences mediated by finite group actions, this current text provides notable insight to some applications and motivations, typically not addressed in histories, either chemical or mathematical.

To facilitate the use of the mathematics described in the text, a general software package has been developed in Kerber's group over the last couple of decades. This package is available *via* internet at <http://www.mathe2.uni-bayreuth.de/axel/symneu.engl.html> and takes advantage of the user shell of MAPLE. The reviewed text, though presenting general mathematics, thence seems of great promise for study by chemists, especially by theoretical or mathematical chemists. Presumably, with the various results covered from the forefront of discrete mathematics there should be further novel chemical applications beyond those made so far. With the increasing interest in combinatorial libraries (indeed so much so that at least two journals dedicated to this area have arisen in the last decade), one might naturally expect that the mathematical ideas developed here may prove of much use in generating and characterizing such libraries, at least when "virtual".