PRIKAZ KNJIGE BOOK REVIEW

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This book provides a comprehensive treatment of the combinatorial theory associated with the symmetry-mediated classification, generation, and enumeration of a variety of discrete mathematical structures. Such structures notably include molecular graphs, geometrical embeddings of graphs, molecular reactions, quantum-chemically symmetry-adapted wave-functions, and a variety of other mathematical graphical and combinatorial species of interest. The group actions may involve point-group symmetries of 3-dimensional structures, and also permutational symmetries corresponding to different fluxional arrangements (as in a non-rigid molecule with internal rotations, inversions, or pseudo-rotations). 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 classifications, 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 perseverence is required of a typical chemical reader. In this regard, chapter 11 surveying some mathematical 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 perseverence seem promising in the generality attained, presumably with many new chemical applications possible.

Notably the text does pay explicit attention to chemistry, as one might suspect from the molecular structural formula for dioxin appearing on the back cover of the book. Chemical applications appear in several points in the text, including:

– some parts of section 2.1 (on »first« enumeration procedures);
– 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 (where the generation of representatives is further illustrated); and
– a surprising amount of the section 12.1 (on the history of the subject of the book).

Thence despite the generality and mathematical framework, there is notable contact to chemistry, and indeed the book really offers a lot of insight to the interconnection between mathematical developments and chemical problems.

General readers may find the historical section 12.1 especially easy to read and of much interest. This section provides a modicum of history of chemical-enumeration methodology such as is typically overlooked in standard histories of chemistry, perhaps because these developments, as by A. Cayley, or by J. J. Sylvester, or by G. Pólya are viewed by many to be more important as developments in mathematics than in chemistry. And indeed these three scientists are recognized as mathematicians, though their work noted in the present book was largely motivated by the chemical applications, to which they made seminal contributions. On the other hand some mathematicians (as Froebenius, Burnside, or Redfield) made important contributions to the indicated area of mathematics while seeming to have been entirely unmotivated and even unaware of chemical applications. Yet others such as N. G. de Bruijn and R. C. Read seem to have had chemistry as a secondary motivation. Notably, as noted in Kerber's book, in the last few decades the theoretical chemist E. Ruch along with his colleagues made fundamental contributions to the mathematical field. Moreover, the work of Kerber and his several students during the last couple of decades seems to have been stimulated by the work of Ruch and his group, so that Kerber's prime motivation may be chemistry, as is further attested to in his service (of more than a decade) as editor of »*Communications in Mathematical Chemistry*«. Of course in the present book one finds some mention of chemists or scientists who did not make detailed mathematical contributions, but rather developed related fundamental chemical concepts. For instance, A. von Humboldt's description of the idea of chemical isomerism in 1799 is noted, though in traditional chemical histories this seems typically to be missed. And also such chemical histories also seem typically to miss entirely the mathematical developments of Cayley, Sylvester, Pólya, and other more recent workers, as are so prominent in Kerber's book. Yet also it seems that the historical points made are typically overlooked in mathematical histories. That is, the historical discussion is quite idiosyncratic, but also it is quite convincing.

Of further interest to chemists are yet further efforts to facilitate the use of the mathematics described in the text. Again there is Kerber's service

as editor of »*Communications in Mathematical Chemistry*«, where related types of articles have been encouraged. But particular notice may be made of a general software package developed (by Kerber's group) over the last couple of decades. This seemingly widely applicable package is available *via* Internet at

http://www.mathe2.uni-bayreuth.de/axel/symneu.engl.html

and takes advantage of a 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. It is to be emphasized that the general attention of the book to the correspondence of the various structures in terms of mappings offers the possibility of doing much more than the classical enumeration. Perhaps subclassifications with a requirement or preclusion of different substructures might be made, and the variety of structures so identified might be efficiently and comprehensively generated. With the increasing interest in combinatorial libraries (indeed so much so that at least two journals focused solely on this area have arisen in the last decade), one might naturally expect that the mathematical ideas developed here have much potential use in generating and characterizing such libraries, at least when »virtual«. It may be concluded that the present mathematics book offers exceptional possibilities for chemical applications.

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