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The Permutation Group in Physics and Chemistry

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Introduction

The permutation group has gained prominence in the fundamental research in diverse areas of physics and chemistry. Covering all salient developments of the last few years in a single symposium would require weeks, legions of participants and parallel sessions, highlighting the differences in language and communication problems between pure mathematicians, high and low energy physicists and chemists. The symposium held July 1978 at the Centre of Interdisciplinary Studies of the University of Bielefeld focussed on a small area, the pertinence of the permutation group in chemical physics, with the goal to increase and generate a fruitful dialogue between mathematicians and chemists.

In chemistry, concerned with the electronic and geometric structure of molecules as well as elementary chemical reactions, i.e. rearrangements in these structures, the permutation group has its relevance, since with its representations the effects and consequences of exchanging indistinguishable particles, electrons and identical nuclei, can be systematized and classified. This may be exemplified by a brief survey of the lectures presented, which may also serve as a first orientation to the articles of this volume. In the first two contributions by A. Kerber and J.G. Nourse, the permutation group is used in the counting and systemtaic generation of stereoisomers aiding in the elucidation of possible molecular structures. The dynamics of stereochemistry is considered in the next article by J.G. Nourse. The following section with four contributions by P.R. Bunker, J.D. Louck, A. Dress and R.S. Berry deals with the permutation group as a generalization of the point group symmetry useful in the interpretation of molecular spectra and structure. This generalization originally suggested by Longuet-Higgings, who unfortunately could not be present at the symposium, provides a frame for the concise description of molecular dynamics with minimal coupling between internal and external motion and is of particular importance when nonrigid molecules are considered. How far this concept can lead is illustrated in the contribution by R.S.Berry, where the full transition of structured molecules to liquid drops is investigated; possibly a guide to a symmetry classification of molecular rearrangements and the kinematics of chemical reactions. The next section with three articles by L.C. Biedenharn, J.D. Louck and B.R. Judd, deal with the representation and classification of electronic wavefunctions for

molecules and atoms using the irreducible representations of the symmetric group as a basis for the description of the spin and angular momentum coupling. How such a symmetry basis can be used effectively for the evaluation of matrix elements, important in the quantitative description of electronic and molecular structure, is illustrated in the contributions by T.H. Seligman and J.S. Frame. This is related to the more recently developed methods for the rapid calculation of configuration mixing matrix elements using the unitary group approach, a topic for a forthcoming special symposium. A final contribution by A. Dress comments on some mathematical aspects of the chirality algebra of Ruch, who was present at and contributed to the symposium.

Finally I would like to use this opportunity to acknowledge the assistance of the organizing committee in the planning of the symposium and express my gratitude to the directorship and staff of the Centre for Interdisciplinary Studies for the financial and organizational assistance, which made the symposium possible. My special thanks go to Mrs. K. Mehandru and B. Yurtsever for the typing of the manuscripts.

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