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book reviews

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Group theoretical methods and applications to molecules and crystals. By Shoon K. Kim. Cambridge: Cambridge University Press, 1999. Pp. xii + 492. Price £95.00. ISBN 0 521 64062 8

According to the author's preface, this book is intended to explain the basic aspects of symmetry groups and their applications to problems in physics and chemistry by using an approach pioneered and developed by the author. The aim is to work out explicitly the structure of symmetry groups and their representations by eliminating the unduly abstract nature of standard group-theoretical methods.

The applied strategy, emphasized by the author, relies upon the fact that all space groups, unitary as well as anti-unitary ones, can be reconstructed from suitably chosen algebraic defining relations of point groups instead of introducing them, as he claims is done in almost all textbooks and monographs on solid-state physics, without any proof as 'god-given'. The matrix representations of space groups are determined by projective representations of their associated point groups, whereas the representations of point groups are subduced from representations of the rotation group. Symmetry-adapted linear combinations of equivalent basis functions transforming according to unitary irreducible representations of point groups are deduced by applying the so-called *correspondence theorem*. This method is used not only to form molecular orbitals and symmetry coordinates of molecules but also to construct the energy-band eigenfunctions of Hamiltonians which are invariant with respect to space groups.

The *Preface* states that the book will be of great interest to graduate students and professionals in solid-state physics, chemistry, mathematics and geology, and especially to those who are interested in magnetic crystal structures.

The book is organized as follows: Chapter 1, *Linear transformations*, discusses the basic concepts of vector spaces and linear transformations and related topics. Chapter 2, *The theory of matrix transformations*, introduces general matrix transformations by putting the main emphasis on so-called involutional transformations. Chapter 3, *Elements of abstract group theory*, describes the basic concepts of groups, subgroups and mappings between groups. Chapter 4, *Unitary and orthogonal groups*, discusses the definition and properties of the unitary group $U(n)$, of the orthogonal groups $O(n, \mathbf{C})$, $O(n, \mathbf{R})$ including the special case $O(3, \mathbf{R})$. Chapter 5, *The point groups of finite order*, lists all possible finite subgroups of the rotation group including their basic properties. Chapter 6, *Theory of group representations*, treats the basic concepts of carrier spaces, like Hilbert spaces, and linear operators, as well as matrix representations of groups by including the properties of irreducible matrix representations. This concept is used to construct, amongst others, symmetry-adapted functions either by means of generating operators or by means of projection operators. Chapter 7, *Construction of symmetry-adapted linear combinations based on the correspondence theorem*, introduces an alternative method for the construction of symmetry-adapted states which is applied to compute hybrid atomic orbitals or, likewise, symmetry coordinates of molecular vibrations. Chapter 8, *Subduced and induced representations*, treats the construction of subduced and induced representations. Special emphasis is put on the situation where the subgroup of a given supergroup is an invariant one, since for all such cases a step-by-step procedure exists that allows the systematic construction of induced representations for the supergroups that are irreducible. Chapter 9, *Elements of continuous groups*, presents some basic aspects, like the parameterization of group elements, the invariant integration, Lie algebras, the connectedness and the multivalued representations of continuous groups. Chapter 10, *The representations of the rotation group*, discusses the structure of the special unitary group $SU(2)$, since the latter is the universal covering group of the special rotation group $SO(3, \mathbf{R})$, which explains why single- and double-valued representations of $SO(3, \mathbf{R})$ exist. Possible representations are realized by introducing generalized spinors and angular momentum eigenfunctions and by using coupling coefficients. In Chapter 11, *Single- and double-valued representations of point groups*, the double-valued representations of point groups are represented by projective representations. As an alternative, ordinary (vector) representations of double point groups are discussed where, apart from the point groups of finite order, the most general point groups of the type C_∞ and D_∞ are considered. Chapter 12, *Projective representations*, introduces the basic concepts of projective representations of groups by demonstrating how covering groups and so-called representation groups are interrelated. Chapter 13, *The 230 space groups*, introduces the basic definition of space groups. Special emphasis is put on the definition of the 14 Bravais lattice types and the 32 crystal classes. These properties are used to define 32 minimal generator sets in order to deduce the 230 space-group types. Chapter 14, *Representations of the space groups*, introduces reciprocal lattices and their Brillouin zones to specify the general induction procedure for the construction of unitary irreducible matrix representations of space groups by favouring the use of projective representations of the underlying point groups. Chapter 15, *Applications of unirreps of space groups to energy bands and vibrational modes of crystals*, uses the free-electron model as the simplest model to construct symmetry-adapted wave functions that are composed of plane waves and transform according to unitary irreducible matrix representations of space groups. To show the different structure of symmetrized wave functions, one example deals with a symmorphic space group, another with the symmetrization of the basis functions with respect to a non-symmorphic space group. The construction of symmetry coordinates of vibration for a crystal with the diamond structure is discussed. Chapter 16, *Time reversal, anti-unitary point groups and their co-representations*, introduces the concept of time-reversal symmetry in classical and quantum mechanics. The definition of so-called anti-unitary point groups together with their co-representations is treated by putting special emphasis on the construction of unitary irreducible co-representations. Chapter 17, *Anti-unitary space groups and their co-representations*, introduces some specific extensions of space groups, here called anti-unitary space groups of the first kind and of the second kind (but presumably better known as Shubnikov or magnetic space groups) by extending the minimal generator sets for space groups correspondingly. The unitary irreducible co-representations of anti-unitary space groups are constructed *via* projective unitary irreducible co-representations of the underlying point groups. As possible applications, selection rules of Hamiltonians that are invariant with respect to anti-unitary space groups are discussed in general terms, but without reference to a single concrete example.

At first glance, on the basis of the concepts presented and the material discussed, the book would seem to qualify as an extremely ambitious project. The merits of the book are that it offers many details on the algebraic properties and matrix representations of point, space and magnetic space groups as well as applications to a number of physical problems such as the symmetry adaptation of functions needed for quantum-mechanical calculations.

Unfortunately, however, a closer look reveals several drawbacks which cause me to hesitate to recommend this book for a wider audience, especially for crystallographers. Full details of these drawbacks are given in the version of this review appearing in the on-line version of the journal. In summary, I note that the mathematical standards are at a rather modest level, perhaps intended by the author so as to improve the book's readability. That, however, remains cumbersome, not only because of the conventions adopted and the notations used, but also because of the great number of misprints. Although the majority of the typographical errors are obvious (and thus the more inexcusable), some of them are extremely misleading as are the several wrong statements the book contains. Apart from that, the book suffers from several conceptual weaknesses such as the general strategy adopted of using results that are stated without a complete proof or proved only in later sections. The book also suffers from a lack of concrete examples as regards the computation of selection rules. Finally, not only the unbalanced list of references must be criticized but a similar lack of balance has to be noted in the treatment of standard group-theoretical problems, as existing alternative methods, well documented in the literature, are entirely ignored.

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