Point Groups, Space Groups, Crystals, Molecules

by R. Mirman

Group Theory: An Intuitive Approach
(Singapore: World Scientific Publishing Co., 1995)

Group Theoretical Foundations of Quantum Mechanics
(Commack, NY: Nova Science Publishers, Inc., 1995)

Massless Representations of the Poincaré Group
electromagnetism, gravitation, quantum mechanics, geometry
(Commack, NY: Nova Science Publishers, Inc., 1995)

Point Groups, Space Groups, Crystals, Molecules
(Singapore: World Scientific Publishing Co., 1999)

Point Groups, Space Groups, Crystals, Molecules

Problem T-1: Finish the diagram.

How is this space group related to that of the cover?

R. Mirman

World Scientific

Singapore • New Jersey • London • Hong Kong

Published by

World Scientific Publishing Co. Pte. Ltd.

P O Box 128, Farrer Road, Singapore 912805

USA office: Suite 1B, 1060 Main Street, River Edge, NJ 07661

UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

POINT GROUPS, SPACE GROUPS, CRYSTALS, MOLECULES

Copyright © 1999 by World Scientific Publishing Co. Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN 981-02-3732-4

Printed in Singapore

Preface

GROUPS, MATHEMATICS, PHYSICS, ART

Group theory is a diverse, extensive subject, playing roles, often fundamental, in numerous areas — there are many different ways in which it is useful, enlightening, often necessary. This book considers thus only a small part of a broad, substantial topic. While a paramount goal is, of course, teaching the theory, certainly providing the basis for application, its deeper rationale is development of (part of) the foundation for the study of group theory more generally, and of mathematics, physics, chemistry, crystallography — and beyond. The hope is to teach group theory, explaining how it is used, not merely that part that it covers — and to nurture the skills to develop and apply it, helping and stimulating the reader to gain thorough understanding.

Group theory is important, essential, for students in many different fields, for many different types of researchers. The book tries to achieve the impossible by appealing to all. It can be used by those only slightly interested, to get a quick definition, a brief introduction to a concept, a slight understanding of what is being read elsewhere, even of only vocabulary. And it can, hopefully, be studied for deeper and deeper understanding, as profound as wished. For those who really study it, who make serious attempts at many of the problems, who think about questions raised, it is designed to develop not only insightful, profound knowledge of groups, and applications, but more generally of mathematics, physics, chemistry, even philosophy. For such readers the desire is to aid also in the development of those skills and habits that lead to success more generally.

How difficult is this book? It is written to be easy to read and understand, for those who want an introduction to the subject, a reading knowledge, fundamental concepts, vocabulary. And it should not be more difficult for readers who wish to go deeper, although of course that requires more work. But it also attempts to provide the material, the questions, the problems, the challenge, the irritation, the skepti-

cism, so that those who wish a very deep understanding, who wish potent skills, and not only in this subject, will have the stimulation and exercises to help obtain them.

Crystals and molecules play a preeminent role in physics and chemistry (and technology and economics), and their groups of transformations are basic in determining their properties and those of objects that compose them. But beyond such applications, they provide subjects quite suited for the development and illustration of many general concepts of group theory, geometry, mathematics. It is thus surprising that there have been so few books devoted to the theory of these groups. There have been (in the past) books available, but there seems to never have been a comprehensive treatment of this quite vast subject. This book is certainly not that, and perhaps such is impossible. But it attempts to at least introduce the major parts of the subject, to show how they are related, and what their importance is — and to provide guidance (certainly references) to those who wish to learn more, to go deeper.

Because of the extent of the subject it is impossible to cover more than a small part. In many cases material is merely mentioned, often in problems, to inform the reader that it exists, to at least provide definitions, and also to indicate where further information can be found. Thus, of regrettable necessity, many topics had to be only outlined, but with references to other discussions, perhaps in more depth. And if the reader should find all these discussions are also only outlines, the conclusions to be drawn would be obvious. Often a topic is referred to only to be able to provide references. Unfortunately these are in too many cases to books no longer in print, frequently long out-of-print. Yet the material that they contain, even just the approach, is often not found anywhere else. As they disappear, the knowledge within them, typically gained with so much difficulty and so useful, disappears also. Thus one hope is to at least keep alive the memory of books long gone, but whose disappearance is a substantial loss. A book at least differs from a person — it can be brought back from the dead. Perhaps if memory can be kept alive, some books themselves might be restored to life.

This book is, of course, aimed at providing knowledge of group theory, to enable its readers (to apply and develop it), specifically the part that deals with discrete, particularly crystallographic, groups, and to use these applications to help in mastering groups, and the systems to which they can be applied. But more, what is emphasized is understanding, intuition, not only about groups, crystals, molecules, but about mathematics, physics, chemistry, crystallography, and related fields, and about understanding. It is designed to push the reader to

understand the theory, the reasons for it, for the properties of (these) groups, for what we have decided should be the properties, and why. So it aims to stimulate, to goad, the reader to think about, not only the material, but its foundations, its reasons, about what is being read. Those in education know that too often we do not educate our students, we program them. Like a good computer program they are able to deal well with material for which they have been programmed. But too often, just as a computer program, they do not understand what they are doing, or why. They do not understand the reasons the particular software has been read into them. They are unable to think about what they are doing, to extend their capabilities to areas other than those for which they have been programmed. Obviously researchers should be able to deal with novelty, but too often they are able to merely apply routinely their built-in software to subjects at most slightly different than those taught to them. And educators also must be able to think innovatively. How else can they teach their students to do so? This is part of the underlying philosophy of the book and the way it was written (like the first book of this series [Mirman (1995a)]). Is the approach correct? Can it achieve what it tries to? Can any approach? This is an experiment. Hopefully it will not only teach the material, and its understanding, to enable readers to deal with it, but also it will teach those who educate a little about how, and about how not, to do so — or at least stimulate (or disturb) them enough so that they will consider these questions. A fundamental rationale is to raise such issues, to prod the reader to think — and to provoke those who use and teach from this book, to also think, not only about group theory, mathematics, physics, but about education. It aims to stimulate others to try to devise ways of better educating, their students and themselves, and hopefully to spread what they have learned, so others may learn, may be sensitized, aroused, so that they too will look — and find — ways of better, not merely programing, but educating.

What is learned in (good) formal education is never sufficient for a successful career. Rather it provides the foundation for necessary further learning. A successful education imparts not only knowledge — necessary for the acquisition of further knowledge — but skills, to go deeper into subjects, to utilize and extend knowledge and skills, to gain further knowledge. It provides not only depth, and the experience to penetrate further, but breadth, flexibility, abilities to go into other fields, to deal with other forms of knowledge, to acquire and use them; it provides the skills necessary to learn other skills.

This is a major aspect of the philosophy of these books. Not only to teach the subjects and the skills to use them, but also those needed to learn more, about these fields, about others, and the capacity to

deal with whatever problems the reader encounters, in whatever fields, however they may arise. For success, especially during uncertainty, breadth and adaptability are essential.

One skill needed by a researcher is judgment — what problems should be attempted? Many problems here are partially trivial, partially research, partially impossible. Deciding what can, and what cannot be done, what is worth trying, is valuable exercise.

Although the question of rigor has been discussed previously [Mirman (1995a), sec. P.5, p. xv], it is worth emphasizing again, for this also is part of the underlying philosophy, and here quite relevant. An exposition is rigorous if it is written in a way so that it can be widely, and easily, understood, thus easily checked. Having been checked by many people, we can be more confident that there are no errors, that all assumptions have been stated. By this standard much of present mathematics and physics is highly nonrigorous. Obscurantism is not rigor, despite the much too popular belief. It is just the opposite.

What is so disturbing is not merely the way much material is so often presented, or written so as not to be presented, but that there is no attempt to explain or understand it. Science becomes a religion; these are the accepted beliefs, there are no reasons for them, there is no need to explain them. Read not only many, but (at least, close to) all, books on these topics. Consider the number of subjects presented, not discussed, without explanation, without justification, without reasons, without understanding, without even the hint of why they are true (if they are), where they came from, or where further discussion or justification can be found (for they cannot). This is not education, it does not lead to understanding. Here then we attempt to fill in (unfortunately, necessarily only some of) these gaps, or at least point them out — and to emphasize how often books on mathematics and science present not explanations, rationales, proofs, but merely beliefs. And very often what everyone believes, while it may be the truth, is not the whole truth. Someone learning the subject should understand this, should know what is true, what is not true, what is not fully true.

For the insightful comprehension we hope the reader will gain, it is important, even essential, to have different views of every (or at least the most important) aspects, and to see how they are related. Thus there are topics covered in great depth. This also allows flexibility. The reader, or the instructor, has available much material from which the choice most fitting for a particular case can be made. There are fewer restrictions because of choices the writer has made.

And to achieve understanding it is necessary to stimulate the reader to think, so to raise questions, doubts even paradoxes, mysteries, contradictions. This underlies many of problems.

While an attempt has been made to explain and justify much material very fully, it is impossible to do this for everything. Much had to be just outlined, with the material taken from standard sources (which are referenced so the reader can find, hopefully, more comprehensive discussions), and many of these took their material from other standard sources. No claim is made that all material taken from such sources has been carefully checked, and perhaps the standard sources did not check everything taken from previous standard sources. It is not unheard-of for errors to be propagated because "facts" become well-known and established, so never checked. Readers should always be very careful. Teaching this is another hope.

Attitudes of researchers, physicists, mathematicians — any researchers — are essential, for success and the production of useful and meaningful work. Of great importance is open-minded skepticism, being willing to examine with care and understanding new ideas, approaches, results no matter how disturbing or contrary to previous beliefs, but also care and skepticism, not only with these but also with accepted beliefs, establishment views. Too many people have instead a closed-minded credulity, closed to anything different from what they are told to believe, but credulous for the sanctioned, the authorized, no matter weakly supported, even absurd, that may be. Too often we accept, uncritically, what we are told, what is on a piece of paper. So the book tries to instill an attitude of open-minded skepticism, to break the connection between appearance of a statement on paper or in a book and acceptance of it. Of course, only slight progress can be made, but it is hoped that at least this is possible — and that others will be stimulated to also try to develop, the so essential, open-minded skepticism. Thus (perhaps too) occasionally, doubts are raised about the statements being presented so to accustom the reader to skepticism, to care, to the habit of checking. Open-mindedness is harder, but perhaps once thought becomes a habit, useful doubt also will.

The philosophy underlying this book is the same as the first one [Mirman (1995a)]. To help the reader understand what is being attempted, an explanation of the approach is attached.

ACKNOWLEDGEMENTS: For much help, this is to thank the Department of Natural Sciences of Baruch College (City University of New York) and World Scientific Publishing Company.

GROUP THEORY: AN INTUITIVE APPROACH

R. Mirman

Level:

First-year graduate, but accessible to many juniors. The right text for a course in group theory (even for undergraduates), as well as a supplementary text for other courses, and for self-study. Valuable also to those working in group theory, or using it in their research. Versatile: provides a quick understanding of a definition, an introduction, or a thorough knowledge and understanding, as desired by the user.

Eminently suitable, as a text, as a developer of skills (including teaching skills), as a reference, as a source of material not available elsewhere, and as a stimulant to thought (pb. VII.7.e-3, p. 213).

Unusual as text; it is designed to teach — to give competitive edge in these difficult times: Its goal is not merely learning, but understanding — group theory and more broadly, physics, mathematics and the application of mathematics to physics. It is written in a style that makes it easy to read, understand, and master. The approach is concrete, coherent, physical, emphasizing motivation (see especially beginning of most chapters), explanation, vocabulary and definitions, and examples (sec. I-6, p. 25; chap. II, p. 29; sec. III-2, p. 68). Problems are stressed, obviously. All the relevant standard ones are here, in one convenient place, usually expanded and elaborated on, plus a vast number of other, original, problems. Valuable to instructors as a source of problems, and for ideas for projects or research.

The book has an educational philosophy (which is unusual); it is based on not only knowledge of group theory and its use in physics gained during many years of research, but also an understanding of the learning process obtained from long experience in teaching. Clearly, the philosophy and approach are original.

Explanatory depth

Explains not only what is happening, but why (sec. I.3.f, p. 10; sec. IV.5, p. 119; sec. X.6.c, p. 292; sec. X.7.e, p. 299). It not merely derives results, but explains why they hold (sec. VI.1.b, p. 171) and how they arise from the assumptions and definitions about groups and representations (sec. VII.5.b, p. 195). What properties of groups, and the objects to which they are applied, give the results being derived (sec. XI.4.a.ii, p. 317; sec. XII.5.b.iii, p. 361)? Why should these hold (sec. IV.5, p. 119)? What do they imply about the mathematics underlying the material, and mathematics in general, and about physics (sec. XI.6, p. 337)? Why are these properties important (sec. VII.3, p. 186)? Illustrations,

examples (throughout the book), even counter-examples (sec. I.3.h, p. 12; pb. III.2.i-4, p. 81; sec. XII.5.e, p. 366), help the reader see what the definitions mean, and understand, remember, and apply them.

Comprehensive: learning different parts of a subject reinforces the rest. The book allows the reader to easily study any topic, strengthening the grasp of all material; and the different parts are explicitly related to each other.

An (unusually) extensive table of contents serves as an outline which organizes material, shows relationships, helps learning, understanding. The style (see, say, the beginning of chapters), also does this.

Definitions and vocabulary

Vocabulary is essential. The book stresses the meaning and significance of terms and concepts (pb. III.4.b-5, p. 87; sec.III.4.e, p. 91; sec.III.4.f, p. 97), making these not only as clear, but as familiar, and easy to remember, as possible. Not only are the terms defined, but often (group-theoretical) reasons for the choice of words are indicated.

Problems improve derivations:

Compare derivations, often uniquely stated, with standard ones (which are also included). Those in other books leave out many steps. While more is put in here, it is neither possible nor desirable to include everything. So many parts are given as problems, reminding the reader that steps are left out and stimulating students to think, and put them in. This is less confusing and makes it easier to understand, learn, and remember the material. And discussions here provide more explanations. Also this helps develop general skills — after working through the book a student will not only know, and understand, group theory, but will be better trained as a mathematician or physicist.

Fruitful as a reference:

Easy to use as a reference, to quickly look up and understand material — without having to read the entire book.

Designed to make finding definitions, explanations, formulas, proofs easy. Very thorough index and table of contents. Extensive and unusually complete cross-references, on almost all pages. Copious citations to other works to provide different views, and indicate where to find material not covered — so assisting readers to expand their capabilities. This is part of its philosophy of not merely presenting material, but educating, helping and encouraging the reader to learn.

Trains (successful) scholars:

The book, perhaps uniquely, is designed to train research mathematicians and physicists, and teachers (pb. I.5.a-7, p. 22; sec. IV.4, p. 116; pb. VII.3.c-1, 2, 3, p. 190; pb. XI.6-4, p. 338). One way is to stimulate them to think (sec. III.6, p. 103), which the entire book tries to do, especially think like a mathematician and physicist (pb. VI.1.b-2, p. 172; p. 181, top; pb. VIII.4.c.ii-1,2, p. 230; pb. XI.4.a.ii-5, p. 318; pb. XII.5-2, p. 358). It is important for a researcher, and especially a teacher, to be able to explain a subject in words (sec. IV.8.c.iii, p. 142). Another aspect of learning mathematics is "art appreciation", to see (and marvel at) the beauty and unity of mathematics, and its application to the physical world (sec. V.5.d, p. 167; sec. IX.2.c, p. 253), and so the beauty of nature. Problems are designed to be thought provoking, to stimulate and teach readers to imagine. And different views of the same subject, the same derivation, not only aid understanding, but teach comparison and evaluation, thus judgment.

Stimulus to research:

Many problems raise questions whose (full) answers are unknown (pb. IV.3.d.iv-9, 10, p. 116; pb. IV.4-18, 19, p. 118; pb. XI.1.a-2, p. 306). It makes easily available important material otherwise difficult to find and organize, and understand, so valuable to those learning, using, and working in group theory, and any of the fields it touches, even people thoroughly familiar with these.

Original:

There is material in the book that appears nowhere else (sec. VI.4, p. 176; sec. X.4.b, p. 281; sec. X.6, p. 287). Much is pedagogical, but some includes proofs or explanations that may not otherwise exist.

The book is unusual, starting with the cover, in ways that make it exceptionally and widely useful, and provocative.

The examples mentioned are only a small sample, as can be seen by looking at almost any page. It is easy to compare the treatment of this book with the corresponding ones of others, where they exist, since complete references are given.

Standards listed are those on which the book should be judged. Compare these to the standards on which other books ask to be judged. People never live up to their standards, but those that they set tell much about them.

World Scientific Publishing Co.

Table of Contents

Preface	v
I Transformations With a Point Fixed: Point Groups	1
I.1 SYMMETRIES OF SPACE AND OF OBJECTS	1
I.2 WHY STRUCTURES OF CRYSTALS AND MOLECULES ARE LIMITED	3
I.2.a What are the essential properties of these objects?	3
I.2.b There are only a few categories of crystals	4
I.3 LATTICES	5
I.3.a Lattices and crystals	6
I.3.b Unit cells	7
I.4 THE ROTATION GROUP AND ITS FINITE SUBGROUPS . . .	8
I.4.a The finite subgroups of the two-dimensional rota- tion group	8
I.4.b The finite subgroups for three-dimensions	8
I.4.c Regular polyhedra	10
I.4.c.i <i>Determination of the regular polyhedra</i>	10
I.4.c.ii <i>Other ways of determining these polyhedra</i>	13
I.4.c.iii <i>Dual polyhedra</i>	15
I.4.c.iv <i>Extensions and generalizations</i>	16
I.4.d How the rotation group determines its finite sub- groups	17
I.4.d.i <i>Orbits and poles and why there are differ- ent types</i>	17
I.4.d.ii <i>The number of orbits and the finite sub- groups</i>	19
I.4.d.iii <i>Implications and extensions</i>	22
I.5 HOW TRANSLATIONS LIMIT ROTATION GROUPS OF CRYSTALS	23
I.5.a Translations limit the trace of the rotation matrix	24
I.5.b Discreteness is essential	25

I.5.c	Complex numbers, rotations and translations . . .	26
I.5.d	Why are rotational symmetries of lattices limited? . . .	27
I.6	POINT GROUPS	27
I.6.a	The symmetry operations on crystals and molecules . . .	28
I.6.a.i	<i>Naming the point symmetry transformations</i>	28
I.6.a.ii	<i>The point symmetry transformations</i>	29
I.6.a.iii	<i>Why only some transformations are considered</i>	33
I.6.b	Naming and describing the point groups	33
I.6.b.i	<i>Point groups with only rotations</i>	35
I.6.b.ii	<i>Restrictions on orders of point groups from their characters</i>	36
I.6.c	Point groups with reflections	39
I.6.c.i	<i>Cyclic groups with reflections</i>	39
I.6.c.ii	<i>Dihedral groups with reflections</i>	40
I.6.c.iii	<i>Adding reflections to the groups of regular polyhedra</i>	41
I.6.d	There are thus 32 point groups	42
I.6.e	Why are these all the point groups?	44
I.6.f	The molecular point groups	46
I.6.g	Objects invariant under the point groups	47
I.7	STRUCTURE OF POINT GROUPS	50
I.7.a	Point groups as semi-direct products	50
I.7.a.i	<i>Dihedral groups</i>	52
I.7.a.ii	<i>Cubic groups</i>	52
I.7.a.iii	<i>The structure of improper point groups</i>	53
I.7.b	Classes of the point groups	55
I.8	DOUBLE GROUPS	57
I.8.a	Definition of double groups	58
I.8.b	Construction of double groups	58
I.8.c	Double group classes	60
I.8.d	The single group is a factor group	62
I.9	SIMPLICITY AND SYMMETRY IN A COMPLEX ENVIRONMENT	64
II	Crystal Structures and Bravais Lattices	66
II.1	CRYSTALS AND LATTICES	66
II.2	LATTICES AND CRYSTAL SYSTEMS	67
II.2.a	Definition of a lattice	68
II.2.b	Unit cells are parallelepipeds	68
II.2.c	What is a Bravais lattice?	69
II.2.d	The holohedry groups and their subgroups	69

II.3	LATTICES IN TWO DIMENSIONS	71
II.3.a	The two-dimensional lattices	71
II.3.b	Why we consider all these lattices, and all distinct	74
II.3.c	Why are points added to unit cells?	75
II.3.d	Where can points be put simultaneously in two dimensions?	76
II.3.e	The symmetry groups of two-dimensional lattices	78
II.3.f	Finding the two-dimensional Bravais lattices analytically	79
II.3.g	What makes two lattices distinct?	80
II.4	THE SEVEN THREE-DIMENSIONAL CRYSTAL SYSTEMS	84
II.4.a	Labeling axes and faces	85
II.4.b	Classification of lattices by their sides and angles	86
II.4.c	Description of the seven systems	86
II.4.d	Why the systems have the names they do	91
II.4.e	The restrictions on projections of lattices from the point groups	92
II.4.f	What determines these systems?	92
II.4.g	Where can axes be placed?	96
II.4.h	What symmetry elements must a lattice contain?	97
II.5	PRIMITIVE AND NON-PRIMITIVE BRAVAIS LATTICES	98
II.5.a	The conditions on added points in three dimensions	98
II.5.a.i	<i>Conditions given by two-dimensional lattices</i>	98
II.5.a.ii	<i>The points allowed by the two-dimensional sublattices</i>	99
II.5.a.iii	<i>Adding points simultaneously</i>	99
II.5.b	Thus there are limits on lattices	102
II.5.c	Finding the Bravais lattices analytically	102
II.6	DESCRIPTIONS OF THE FOURTEEN LATTICES	103
II.6.a	Triclinic, monoclinic, orthorhombic and tetragonal systems	103
II.6.b	The cubic system	105
II.6.c	The trigonal and hexagonal systems	107
II.6.d	The rhombohedral unit cell	108
II.7	THE SEVEN CRYSTAL SYSTEMS AND THEIR SYMMETRY GROUPS	111
II.7.a	Systems, groups and lattices	112
II.7.b	Derivation of the Bravais lattices from their symmetry	113
II.7.b.i	<i>The monoclinic lattices</i>	113
II.7.b.ii	<i>Tetragonal lattices</i>	114
II.7.b.iii	<i>The orthorhombic lattices</i>	116
II.7.b.iv	<i>The trigonal and hexagonal lattices</i>	118

II.7.b.v	<i>The cubic system</i>	119
II.7.c	Seven lattice symmetry groups and fourteen lattices	120
II.7.d	Decreasing the symmetry	120
II.7.e	Dilatations relating lattices	121
II.7.f	Crystals and lattices	121
II.8	THE SYMMETRIES OF CUBIC AND HEXAGONAL LATTICES	126
II.8.a	The rotational symmetries of the cube	126
II.8.b	The symmetry group as a subgroup of symmetric groups	127
II.8.c	The representation matrices of the symmetry group	128
II.8.d	Adjunction of the inversion	129
II.8.e	Generalizations of the cube	129
II.8.f	The symmetries of the hexagonal lattice	130
III	Space Groups	132
III.1	GROUPS WITH DISCRETE TRANSLATIONS	132
III.2	SPACE GROUPS: DEFINITIONS AND NOTATIONS	133
III.2.a	Denoting space group operations	134
III.2.b	The affine group	134
III.2.c	Types of space groups	135
III.2.d	Translations are invariant	135
III.2.e	Semi-direct products	136
III.3	SYMMORPHIC SPACE GROUPS	137
III.3.a	A symmorphic group in two-dimensions	138
III.3.b	Glide planes	140
III.4	NONSYMMORPHIC SPACE GROUPS	141
III.4.a	Screw axes	142
III.4.a.i	<i>The space group with a screw and the point group</i>	144
III.4.a.ii	<i>Limitations on crystallographic screws</i>	145
III.4.a.iii	<i>Pairs of enantiomorphic screws</i>	146
III.4.b	The nonprimitive glide reflection	146
III.4.c	Why are these the only non-primitive operations?	148
III.4.c.i	<i>These are the — only — nonprimitive op- erations</i>	149
III.4.c.ii	<i>Nonprimitive operations are determined by primitive ones</i>	151
III.4.d	The factor group of a space group gives a point group	152
III.4.d.i	<i>Cosets and coset representatives</i>	153

III.4.d.ii	<i>The difference in factor groups of sym-</i> <i>morphic and nonsymmorphic groups . . .</i>	154
III.4.e	How nonprimitive elements are restricted	154
III.4.f	Example of a two-dimensional nonsymmorphic group	156
III.4.f.i	<i>How the crystal differs from the lattice . .</i>	157
III.4.f.ii	<i>The space group operations</i>	157
III.4.f.iii	<i>Shifting the origin cannot make the group</i> <i>symmorphic</i>	158
III.5	THE DIAMOND STRUCTURE	159
III.5.a	The point group of the diamond space group . . .	162
III.5.b	Where are the nonprimitive elements placed? . . .	164
III.5.b.i	<i>Placing glides</i>	164
III.5.b.ii	<i>Placing screws</i>	164
III.5.c	Why is the space group of diamond so rich? . . .	165
III.5.d	Spinel	166
III.6	INHOMOGENEOUS ROTATION GROUPS AND NONSYM-	
	MORPHIC GROUPS	167
III.6.a	Are nonsymmorphic space groups semi-direct prod-	
	ucts?	168
III.6.b	Why are there nonsymmorphic groups?	168
III.7	GEOMETRIC AND ARITHMETIC EQUIVALENCE OF CRYSTAL	
	CLASSES	169
III.8	THE SPACE GROUPS IN ONE AND TWO DIMENSIONS . . .	172
III.8.a	The symmetry groups of linear objects (frieze groups)	173
III.8.b	Space groups with two translations	175
III.8.b.i	<i>Description of the two-dimensional space</i> <i>groups</i>	176
III.8.b.ii	<i>Notation and illustrations for the wallpa-</i> <i>per groups</i>	178
III.9	THE THREE-DIMENSIONAL SPACE GROUPS	180
III.9.a	The symmorphic space groups	180
III.9.a.i	<i>Ambiguities of setting give more space</i> <i>groups</i>	181
III.9.a.ii	<i>Why are these the symmorphic space</i> <i>groups?</i>	181
III.9.b	Enantiomorphic space groups	182
III.9.c	Deriving the space groups by enumeration	182
IV	Representations of Translation Groups	185
IV.1	REPRESENTATIONS AND THE ROLE THEY PLAY	185
IV.2	REPRESENTATIONS OF TRANSLATIONS	186

IV.2.a	The reciprocal space	186
IV.2.b	Lattice points and vectors	188
IV.2.c	Brillouin zones	189
IV.2.c.i	<i>Brillouin zones are of the lattice</i>	190
IV.2.c.ii	<i>Symmetry of points in the Brillouin zone</i>	190
IV.2.c.iii	<i>Boundaries of Brillouin zones</i>	191
IV.2.c.iv	<i>Examples of two-dimensional Brillouin zones</i>	192
IV.2.d	The representation basis states of the translations	193
IV.2.e	Bloch's theorem	193
IV.2.f	The translation irreducible representations	194
IV.3	THE WIGNER-SEITZ CELLS	196
IV.3.a	The centered rectangular lattice — what determines its cell?	197
IV.3.b	The space-filling parallelohedra	199
IV.3.c	Dual figures	201
IV.3.d	Inscription in, and circumscription about, spheres	201
IV.3.e	Illustrations of parallelohedra	202
IV.3.f	Parallelohedra give lattices	203
IV.3.g	Determining parallelohedra from their properties	204
IV.3.g.i	<i>The two-dimensional projections of the cells</i>	204
IV.3.g.ii	<i>The cells are centrosymmetric</i>	205
IV.3.g.iii	<i>The faces form bands</i>	205
IV.3.g.iv	<i>Sharing by adjacent cells</i>	207
IV.3.g.v	<i>Counting nearest neighbors</i>	207
IV.3.h	The number of sides of parallelohedra	210
IV.4	LATTICES CAN HAVE SEVERAL WIGNER-SEITZ CELLS	212
IV.4.a	Emphasizing the importance of understanding what is geometry, what is convention	212
IV.4.b	The centered tetragonal lattice	213
IV.4.c	Implications of multiple Wigner-Seitz cells	214
IV.5	WIGNER-SEITZ CELLS FOR THE LATTICES	215
IV.5.a	The cubic system	216
IV.5.a.i	<i>The simple cube</i>	216
IV.5.a.ii	<i>The face-centered cubic lattice</i>	216
IV.5.a.iii	<i>The body-centered cubic lattice</i>	218
IV.5.b	The tetragonal system	221
IV.5.b.i	<i>The primitive tetragonal lattice</i>	221
IV.5.b.ii	<i>The tetragonal Wigner-Seitz cell is not a stretched cubic Wigner-Seitz cell</i>	222
IV.5.b.iii	<i>The body-centered tetragonal lattice</i>	223
IV.5.b.iv	<i>The all-face-centered lattice</i>	224

IV.5.b.v	<i>Why the tetragonal has fewer lattices than the cubic</i>	224
IV.5.b.vi	<i>The differing Wigner-Seitz cells of the lattice</i>	226
IV.5.b.vii	<i>How cells change</i>	227
IV.5.b.viii	<i>Surfaces appear when edges disappear</i>	229
IV.5.b.ix	<i>Cells as limits of others</i>	230
IV.5.c	The orthorhombic system	230
IV.5.c.i	<i>The simple orthorhombic lattice</i>	231
IV.5.c.ii	<i>The two-face-centered orthorhombic lattice</i>	231
IV.5.c.iii	<i>The all-face-centered orthorhombic lattice</i>	232
IV.5.c.iv	<i>The body-centered orthorhombic lattice</i>	232
IV.5.d	The other systems	234
IV.5.e	Why are there five categories of Wigner-Seitz cells?	235
IV.5.f	Obtaining three-dimensional cells from their cross-sections	237
IV.5.g	Lattices as spaces and representations of their translation groups	238
IV.6	BRILLOUIN ZONES FOR THE LATTICES	239
IV.6.a	The cube and its relatives	240
IV.6.a.i	<i>The Brillouin zone of the simple cube</i>	240
IV.6.a.ii	<i>The Brillouin zone of the body-centered cubic lattice</i>	241
IV.6.a.iii	<i>The Brillouin zone of the face-centered cubic lattice</i>	242
IV.6.b	The Brillouin zones of the tetragonal lattices	243
IV.6.c	The other systems	245
V	Representations: Point Groups and Projective	247
V.1	FORMULATING REPRESENTATIONS	247
V.2	REPRESENTATIONS OF THE CRYSTALLOGRAPHIC POINT GROUPS	247
V.2.a	The characters of point groups	248
V.2.b	Representations and characters of cyclic groups	248
V.2.c	Dihedral group representations and characters	249
V.2.d	Computation of characters	251
V.2.e	The table of characters	254
V.2.f	Representations of the tetrahedral and octahedral groups	255
V.2.g	Adjunction of reflections and the inversion	256
V.3	REPRESENTATIONS OF DOUBLE GROUPS	256

V.3.a	The representations of the double cyclic groups	257
V.3.b	Representations of D_2^*	258
V.3.c	Representations of other double groups	259
V.4	PROJECTIVE REPRESENTATIONS	259
V.4.a	Definition of projective representation	260
V.4.b	Factor systems	261
V.4.b.i	<i>The multiplier</i>	262
V.4.b.ii	<i>The Abelian group formed by the factor classes</i>	262
V.4.b.iii	<i>All factors give projective representations</i>	263
V.4.b.iv	<i>The factors are roots of unity</i>	265
V.4.b.v	<i>Properties of factor systems and projective representations</i>	266
V.4.c	Some groups with projective representations	267
V.4.c.i	<i>Projective representation of cyclic groups and products</i>	267
V.4.c.ii	<i>Dihedral groups</i>	269
V.5	CENTRAL EXTENSIONS	270
V.5.a	Nonuniqueness of central extensions	271
V.5.a.i	<i>Symmetric group S_3 as a central extension</i>	271
V.5.a.ii	<i>Why central extensions are not unique</i>	272
V.5.a.iii	<i>Central extension of the four-group</i>	272
V.5.b	Central extensions and factor systems	274
V.5.b.i	<i>The multiplier and central extensions</i>	276
V.5.b.ii	<i>The meaning of projective representation</i>	276
V.5.b.iii	<i>The covering group</i>	277
V.5.b.iv	<i>Why only one factor system is considered</i>	277
V.5.c	Forming a central extension using a specific factor system	277
VI	Induced Representations	280
VI.1	INDUCING AND SUBDUCING TO FIND REPRESENTATIONS	280
VI.2	SUBDUCED REPRESENTATIONS	281
VI.2.a	Conjugate representations	281
VI.2.b	Orbit of a representation	283
VI.2.c	Little groups	284
VI.2.d	The multiplicity of an orbit is representation independent	286
VI.2.e	There is but one orbit in the decomposition	287
VI.2.f	The set of subduced representations of a normal subgroup — Clifford's theorem	288
VI.3	INDUCED REPRESENTATIONS	288

VI.3.a Representation finding using induction	289
VI.3.b Definition of induced representation	291
VI.3.c The matrices give a representation of the group	292
VI.4 EXAMPLES OF INDUCED REPRESENTATIONS	293
VI.4.a Representations of S_3 as examples of induction	294
VI.4.b Induced representations of D_4	298
VI.4.c The representations of tetrahedral group $T (A_4)$	301
VI.4.d Induced representations of octahedral group O	303
VI.4.e Inducing from a nonnormal subgroup	305
VI.4.f Representations of S_4 from S_3	306
VI.5 PROPERTIES OF INDUCED REPRESENTATIONS	308
VI.5.a Basis functions of induced representations	308
VI.5.b Conjugate representations, little groups, and orbits	312
VI.5.c Conjugate subgroups	313
VI.5.d The characters of the induced representation	314
VI.5.e The Frobenius reciprocity theorem	317
VI.6 IRREDUCIBILITY AND COMPLETENESS FOR ARBITRARY SUBGROUPS	319
VI.7 INDUCING FROM A NORMAL SUBGROUP	321
VI.7.a Proof of irreducibility of the induced representation	322
VI.7.b Irreducibility of representations induced from nor- mal subgroup	323
VI.7.c Allowable representations of the little group	324
VI.7.d All representations are given by the allowable rep- resentations	325
VI.7.e Obtaining only nonequivalent representations	327
VI.7.f Finding the induced representation using the little group	327
VI.7.g The matrices of the induced representations	328
VI.7.h Induced representations of direct product groups	329
VI.7.i Semi-direct product groups	330
VI.7.i.i Cases for which induced representations can be found as Kronecker products	331
VI.7.i.ii The representations that are of the form of Kronecker products	332
VI.7.i.iii Subgroups with indices 2	335
VII Representations of Space Groups	337
VII.1 FINDING THE REPRESENTATIONS	337
VII.2 CONCEPTS FOR THE REPRESENTATIONS	338

VII.2.a	The type of space group representations studied here	339
VII.2.b	Induced representations in the terminology of space groups	340
VII.2.c	Orbits	341
VII.2.d	The star of a vector	342
VII.2.e	Classification of positions of Brillouin zones	342
VII.2.f	The cosets formed from the translations	343
VII.2.g	Little groups and reciprocal lattice vectors	343
VII.2.h	Little co-groups and little groups	344
VII.3	REPRESENTATIONS OF LITTLE GROUPS AND LITTLE CO-GROUPS	347
VII.3.a	Small representations, and why they help	347
VII.3.a.i	<i>Translation representations are scalars in little groups</i>	348
VII.3.a.ii	<i>Representations can be obtained from the little co-group</i>	349
VII.3.a.iii	<i>The induced representation matrices</i>	350
VII.3.a.iv	<i>The point group part of the matrices</i>	351
VII.3.b	The central extensions of the little co-group	351
VII.3.c	Symmorphic space groups	352
VII.4	INDUCING REPRESENTATIONS OF NONSYMMORPHIC SPACE GROUPS	353
VII.4.a	Representations, allowable and not	353
VII.4.b	Inducing representations of symmorphic space groups	354
VII.4.c	Representations of nonsymmorphic groups	355
VII.4.c.i	<i>These matrices form a representation</i>	357
VII.4.c.ii	<i>The representations are irreducible</i>	357
VII.4.c.iii	<i>All inequivalent representations are obtained</i>	359
VII.4.d	The allowable representations of the little group	359
VII.4.d.i	<i>Obtaining the allowable representations from representations of the little co-group</i>	359
VII.4.d.ii	<i>The cases of internal vectors</i>	361
VII.4.d.iii	<i>Special positions on the boundary</i>	361
VII.5	WHAT THE PROCEDURE IS, AND WHAT IT MEANS	364
VII.5.a	The procedure in essence	364
VII.5.b	What operators are diagonal?	365
VII.5.c	The meaning of space group representations	367
VII.5.d	What is the dimension of the space group representation?	369

VII.5.e	Representations can contain more than one momentum magnitude value	370
VII.6	THE SQUARE AS AN EXAMPLE	372
VII.6.a	The reciprocal lattice vectors of the square . . .	372
VII.6.b	General vectors and vectors giving symmetry . .	372
VII.6.c	The stars of the points of the square	373
VII.6.d	The square and the rectangle	376
VII.6.e	Little groups of general, and of special, vectors .	377
VII.6.f	Representations of the space group of the square	377
VII.6.f.i	<i>The little groups and the representations</i> . . .	377
VII.6.f.ii	<i>What determines the little groups?</i>	379
VII.6.g	The square with nonsymmorphic glides	379
VII.6.h	A nonsymmorphic group of the rectangle	380
VII.6.i	What determines the space group and its representations?	383
VII.6.i.i	<i>The representation basis functions</i>	383
VII.6.i.ii	<i>How the glide affects basis functions</i>	384
VII.7	THE CUBIC AND DIAMOND STRUCTURES	384
VII.7.a	The representations of the factors for $Fm\bar{3}m$. . .	389
VII.7.b	The representations of the factors for $Fd\bar{3}m$. . .	389
VII.7.b.i	<i>Representations at Point Γ</i>	390
VII.7.b.ii	<i>Points with nonsymmorphic little groups</i> . .	391
VIII	Spin and Time Reversal	393
VIII.1	MORE COMPLICATED CRYSTALS	393
VIII.2	TIME REVERSAL	394
VIII.2.a	Antilinear and antiunitary operators	395
VIII.2.b	The general form of an antilinear operator . . .	396
VIII.2.c	The general form of the time reversal operator .	398
VIII.2.d	Kramer's Theorem	402
VIII.3	COMPLEX CONJUGATE REPRESENTATIONS	403
VIII.3.a	When are conjugate representations equivalent? .	403
VIII.3.b	Operators mixing representations and their conjugates	404
VIII.3.c	Classification of groups under complex conjugation	405
VIII.3.c.i	<i>Potentially real, and pseudo-real, representations</i>	405
VIII.3.c.ii	<i>Ambivalent groups and their character sets</i>	406
VIII.3.c.iii	<i>Why physically are groups so classified?</i> . . .	407
VIII.3.c.iv	<i>Reality and the rotation group</i>	409

VIII.3.d Equivalent sets can be distinguishable	410
VIII.3.d.i <i>Mathematical equivalence, and physical equivalence</i>	411
VIII.3.d.ii <i>Complexity of half-integral angular momentum statefunctions</i>	411
VIII.4 COLOR GROUPS	411
VIII.4.a The conditions on color groups	413
VIII.4.b Point groups with time reversal	414
VIII.4.b.i <i>Cyclic color groups</i>	415
VIII.4.b.ii <i>Dihedral color groups</i>	416
VIII.4.b.iii <i>Gray groups</i>	418
VIII.4.c Magnetic groups	419
VIII.4.d An example of a magnetic group	421
VIII.4.e Construction of a magnetic group	421
VIII.4.e.i <i>The square has other magnetic groups</i>	422
VIII.4.e.ii <i>Why the square has these magnetic groups</i>	422
VIII.4.f The orthorhombic magnetic crystal	424
VIII.4.g What determines which groups are different?	426
VIII.5 MAGNETIC BRAVAIS LATTICES	426
VIII.5.a Properties of the magnetic Bravais lattices	428
VIII.5.b Two-dimensional magnetic Bravais lattices	429
VIII.5.c Three-dimensional magnetic Bravais lattices	429
VIII.6 MAGNETIC SPACE GROUPS	431
VIII.6.a Types of colored space groups	432
VIII.6.b A space group obtained from the primitive cubic lattice	433
VIII.6.c Implications and extensions	433
VIII.7 REPRESENTATIONS OF GROUPS WITH ANTILINEAR OPERATORS	434
VIII.7.a Corepresentations	435
VIII.7.b Multiplication rules for corepresentations	436
VIII.7.c Representation Spaces	437
VIII.7.d Constructing the corepresentations	437
VIII.7.e Transformations of the corepresentations	440
VIII.7.f Reducibility of corepresentations	441
VIII.7.g The types of corepresentations	441
VIII.7.h The case of inequivalent subgroup representations, Δ and Δ^+	442
VIII.7.i Equivalent subgroup representations	443
VIII.7.i.i <i>Transforming to reduced form</i>	444
VIII.7.i.ii <i>The case with the sign positive</i>	446
VIII.7.i.iii <i>The case with the minus sign</i>	447

VIII.7.j	A simple corepresentation	448
VIII.7.k	Which representations are which?	449
VIII.7.l	The Herring test	451
VIII.7.m	Are corepresentations representations?	453
VIII.8	SPIN AND COREPRESENTATIONS	454
VIII.8.a	Integral spin	454
VIII.8.b	Half-integer spin	454
VIII.8.c	Classifying the corepresentations	455
VIII.9	APPLICATION OF COREPRESENTATIONS TO MAGNETIC SPACE GROUPS	456
VIII.9.a	The translation operators	456
VIII.9.b	Corepresentations of the magnetic space groups	457
VIII.9.b.i	<i>The procedure for unitary groups</i>	457
VIII.9.b.ii	<i>How the procedure is changed for mag- netic space groups</i>	458
VIII.9.c	Projective corepresentations of magnetic groups	459
VIII.9.d	Time reversal invariance and gray space groups	462
VIII.9.d.i	<i>Unitary magnetic little groups</i>	462
VIII.9.d.ii	<i>Magnetic little groups with antiunitary operators</i>	463
VIII.9.d.iii	<i>Degeneracies depend on the magnetic corepresentation</i>	463
VIII.9.e	The physical meaning of the representations	463
VIII.10	REPRESENTATIONS OF DOUBLE SPACE GROUPS	464
IX	Tensors, Groups and Crystals	467
IX.1	MACROSCOPIC PHYSICAL PROPERTIES OF CRYSTALS	467
IX.2	TENSORS FOR THE ROTATION GROUPS	468
IX.2.a	The number of representations symbolized by a tensor	469
IX.2.b	Pseudo-tensors	473
IX.2.b.i	<i>Tensors formed from products of vectors</i>	473
IX.2.b.ii	<i>Restrictions on crystal properties</i>	474
IX.2.c	Tensors relating vectors	474
IX.2.d	Required symmetry in indices	475
IX.3	TENSORS AND SYMMETRY	476
IX.3.a	Foundations of the tensor analysis of crystal prop- erties	477
IX.3.a.i	<i>Neumann's principle</i>	477
IX.3.a.ii	<i>Is Neumann's principle obvious?</i>	478
IX.3.a.iii	<i>Why tensor components are point-group scalars</i>	479
IX.3.b	Equilibrium and non-equilibrium properties	480

IX.3.c	Magnetic tensors and the effect of time reversal	481
IX.3.d	The number of independent components	481
IX.3.e	The meaning of the number of independent components	484
IX.3.f	Requirements imposed by symmetry elements on tensors	484
IX.3.g	How group theory provides information about tensors	487
IX.4	RANK-1 TENSORS — ELECTRIC AND MAGNETIC DIPOLE MOMENTS	487
IX.5	SECOND RANK TENSORS	489
IX.5.a	Thermal conductivity	489
IX.5.a.i	<i>The meaning of the symmetric and anti-symmetric parts</i>	490
IX.5.a.ii	<i>The physical quantities given by the symmetric parts</i>	491
IX.5.b	Thermal expansion	492
IX.5.c	Stress and strain	494
IX.5.d	Second-rank tensors for group C_{3v}	495
IX.5.e	Nonzero components for different crystal systems	496
IX.6	THIRD-RANK TENSORS	497
IX.6.a	Piezoelectricity	497
IX.6.b	The Hall effect	498
IX.6.c	Optical activity	499
IX.6.d	Groups that can, and cannot, have these tensor properties	500
IX.7	FOURTH RANK TENSORS	501
IX.7.a	Relating stress and strain	501
IX.7.b	Photoelasticity	503
IX.8	THE EFFECT OF IRREDUCIBILITY ON THE PHYSICS OF TENSORS	505
IX.9	THE USEFULNESS OF TENSORS IN ANALYZING CRYSTALS	511
X	Groups, Vibrations, Normal Modes	512
X.1	WHAT GROUPS TELL US ABOUT MOLECULES AND CRYSTALS	512
X.2	VIBRATIONAL STATES AND SYMMETRY	513
X.2.a	Normal modes	514
X.2.b	The simple harmonic oscillator	516
X.2.c	Group theory of the one-dimensional simple harmonic oscillator	517

X.2.d	The linear triatomic molecule	518
X.3	WHY, AND HOW, GROUP THEORY IS RELEVANT TO VIBRATIONS	520
X.3.a	Symmetry and normal coordinates	522
X.3.a.i	<i>Kinetic energy, potential energy and normal coordinates</i>	523
X.3.a.ii	<i>Proof of the existence of normal coordinates</i>	525
X.3.b	Finding normal coordinates	526
X.3.b.i	<i>Valence bond lengths and interbond angles</i>	527
X.3.b.ii	<i>Coordinates that are not independent</i>	527
X.4	CHARACTERS AND COUNTING	528
X.5	EXAMPLES OF APPLICATION OF SYMMETRY TO VIBRATIONS	529
X.5.a	Group theory, symmetry and the vibrations of water	530
X.5.a.i	<i>The vibrational representations</i>	531
X.5.a.ii	<i>The symmetry coordinates</i>	533
X.5.a.iii	<i>Internal coordinates for water</i>	536
X.5.b	Ammonia	537
X.5.b.i	<i>The vibrational representations</i>	538
X.5.b.ii	<i>Displacements in the normal modes</i>	539
X.5.b.iii	<i>The two-dimensional E modes</i>	541
X.5.b.iv	<i>Internal coordinates for ammonia</i>	542
X.5.b.v	<i>Why is group theory relevant here?</i>	543
X.5.c	How vibrational spectra depend on the molecule	544
X.5.d	Breaking of symmetry	549
X.6	MULTIPLE EXCITATIONS	550
X.7	TRANSITIONS AND SELECTION RULES	552
X.7.a	Transitions due to electric dipole moments	554
X.7.b	Polarizability and the Raman effect	556
X.7.b.i	<i>Raman scattering is of second order</i>	556
X.7.b.ii	<i>The angular-momentum selection rules</i>	557
X.7.b.iii	<i>Exclusion rule</i>	558
X.7.b.iv	<i>Raman scattering for crystals</i>	558
X.8	HOW REASONABLE ARE THE APPROXIMATIONS?	559
X.9	HOW DIFFERENT GROUPS GIVE DIFFERENT VIBRATIONAL SPECTRA	561

XI Bands, Bonding, and Phase Transitions	564
XI.1 WHY IS SYMMETRY RELEVANT?	564
XI.1.a Different types of objects can be studied separately	565
XI.1.b Degeneracy, necessary and accidental	566
XI.1.c What can we know about objects in crystals?	566
XI.1.d Symmetry varies; how is it useful?	567
XI.1.e Selection rules, perhaps not exact, but still productive	569
XI.2 ELECTRON STATES IN CRYSTALS	569
XI.2.a Labels for states are necessary	570
XI.2.b Bands, and why they are	570
XI.2.c What group theory tells about electron bands	571
XI.2.c.i <i>Point groups differ at different points in reciprocal space</i>	572
XI.2.c.ii <i>How these bands illustrate the meaning of space group representations</i>	573
XI.2.d Symmetry reduction	574
XI.2.e The equation governing the objects	576
XI.2.f Translational symmetry and bands	577
XI.2.g Energy eigenvalues	578
XI.2.h Energies and statefunctions for cubic lattices	579
XI.2.h.i <i>The simple cubic lattice</i>	579
XI.2.h.ii <i>The body-centered cubic lattice</i>	584
XI.2.h.iii <i>The face-centered cubic lattice</i>	585
XI.2.i Energy bands for nonsymmorphic groups	586
XI.2.i.i <i>Sticking together of bands</i>	586
XI.2.i.ii <i>Irreducible representations on the zone faces</i>	587
XI.2.i.iii <i>The little group need not be a subgroup of the point group</i>	589
XI.2.j The close-packed hexagonal structure	590
XI.2.j.i <i>Nonsymmorphic elements of the crystal</i>	590
XI.2.j.ii <i>Special positions of the Brillouin zone</i>	592
XI.2.j.iii <i>Representations, and the effect of nonsymmorphic elements</i>	594
XI.2.k What do we learn from this group-theoretical analysis?	596
XI.3 THE EFFECT OF TIME REVERSAL	596
XI.3.a The energy surfaces must have inversion symmetry	597
XI.3.b Degeneracy due to time reversal	597
XI.3.c Degeneracy at general points	598

XI.4 LATTICE VIBRATIONS	598
XI.4.a The dynamical matrix	600
XI.4.b Transitions in the simple cubic lattice	600
XI.5 ATOMS IN CRYSTALS AND ENERGY LEVEL SPLITTING	601
XI.5.a Level splitting in crystals	601
XI.5.a.i <i>Some different possibilities</i>	602
XI.5.a.ii <i>Steps in the decomposition</i>	602
XI.5.b The octahedral group as an example	603
XI.5.b.i <i>The intermediate case</i>	603
XI.5.b.ii <i>The case of a weak crystal field</i>	605
XI.5.b.iii <i>Splitting of the octahedral levels</i>	605
XI.6 SPIN-ORBIT COUPLING	606
XI.6.a Spin-orbit coupling and removal of degeneracy	606
XI.6.b Cubic symmetry	607
XI.7 MOLECULAR ORBITALS	607
XI.7.a Relating molecular orbitals and atomic orbitals	608
XI.7.b The types of orbitals we consider	609
XI.7.c Benzene	610
XI.7.d Bonding and antibonding states	611
XI.7.d.i <i>Tetrahedral carbon</i>	611
XI.7.d.ii <i>Trigonal carbon</i>	612
XI.8 CHANGE OF PHASE	613
XI.8.a First and second order phase transitions	613
XI.8.b Limitations on the analysis	615
XI.8.c Specifying the crystal thermodynamics	616
XI.8.d Equilibrium	616
XI.8.e How symmetry change is found	617
XI.8.f The order parameter	618
XI.8.f.i <i>Magnetic ordering</i>	618
XI.8.f.ii <i>Alloys</i>	619
XI.8.g Expansion of the density	620
XI.8.h Physically irreducible representations	622
XI.8.i Symmetry restrictions on the expansion coefficients	622
XI.8.j Implications of the requirement that Φ be a minimum	624
XI.8.k Conditions from necessity of terms being zero	625
XI.8.k.i <i>The third-order term must be zero</i>	625
XI.8.k.ii <i>The fourth-order term</i>	626
XI.8.k.iii <i>The requirement of spatial homogeneity</i>	626
XI.8.l Halving the symmetry always allows a transition	627
XI.8.m Active and passive representations	627

XL9 CLASSICAL VIEWS, QUANTUM VIEWS, REALITY	627
A Symbols and definitions	630
B The Point Groups	631
C Objects Invariant Under the Point Groups	637
D Two-Dimensional Space Groups	650
E Point Group Character Tables	655
E.1 DENOTING THE REPRESENTATIONS	655
E.2 THE CHARACTER TABLES	656
References	674
Index	683

List of Tables

I.4.c.i-1	REGULAR POLYHEDRA	13
I.4.d.ii-1	FINITE SUBGROUPS OF $SO(3)$	21
IV.3.b-1	PARAMETERS FOR THE PARALLELOHEDRA	200
IV.3.c-1	PARALLELOHEDRA AND THEIR DUALS	201
V.2.d-1	CONTRIBUTIONS TO CHARACTERS	252
V.3.a-1	REPRESENTATIONS OF C_2^*	257
V.3.b-1	CHARACTERS OF D_2^*	258
VII.6.e-1	GROUPS OF $\underline{k}$	377
VII.7-1	PARAMETERS FOR POINTS OF O_h^5 AND O_h^7	386
VII.7-2	PARAMETERS FOR LINES OF O_h^5 AND O_h^7	386
VII.7-3	PARAMETERS FOR PLANES OF O_h^5 AND O_h^7	387
B-1	CRYSTALLOGRAPHIC POINT GROUP GENERATORS .	633
B-2	THE CRYSTALLOGRAPHIC POINT GROUPS	634
E.1-1	CONVENTIONS FOR THE REPRESENTATIONS	656
E.2-1	THE CHARACTERS OF THE POINT GROUPS	657

List of Figures

I.3-1	LATTICE VECTORS	5
I.4.c.i-1	PROJECTED ANGLES	11
I.4.c.i-2	VERTEX ANGLES	11
I.4.d.i-1	SYMMETRY AXES OF A CUBE	18
I.4.d.i-2	ROTATION OF A CUBE BY $\frac{2\pi}{3}$	19
I.5.b-1	EXAMPLES OF ALLOWED ROTATIONS	25
I.5.b-2	HOW OTHER CASES FAIL	25
I.6.a.ii-1	TRANSFORMATIONS OF A HAND	30
I.6.a.ii-2	TRANSFORMATIONS OF COORDINATE AXES . . .	31
I.7.a.ii-1	TETRAHEDRON INSCRIBED IN A CUBE	52
II.3.b-1	CENTERED RECTANGULAR LATTICE	74
II.3.b-2	SYMMETRY OF THE HEXAGON	75
II.3.c-1	CENTERED HEXAGON	76
II.3.d-1	WHERE POINTS CAN, AND CANNOT, BE PLACED .	77
II.4.c-1	MONOCLINIC UNIT CELL	87
II.4.c-2	ORTHORHOMBIC LATTICE UNIT CELL	88
II.4.c-3	RHOMBOHEDRAL UNIT CELL	89
II.4.c-4	THE HEXAGONAL LATTICE	90
II.4.f-1	DROPPING RESTRICTIONS CHANGES LATTICES .	94
II.4.f-2	CUBE GOES TO A RHOMBOHEDRON	94
II.5.a.iii-1	TWO-FACE CENTERING IS IMPOSSIBLE	100
II.6.a-1	TRICLINIC UNIT CELL	103
II.6.a-2	MONOCLINIC UNIT CELLS	104
II.6.a-3	UNIT CELLS OF THE ORTHORHOMBIC SYSTEM . .	105
II.6.a-4	UNIT CELLS OF THE TETRAGONAL SYSTEM . . .	105
II.6.b-1	UNIT CELLS OF THE CUBIC SYSTEM	105
II.6.b-2	THE CUBIC SYSTEM WITH DISTINCT VERTICES .	107
II.6.d-1	RHOMBOHEDRAL UNIT CELL	108
II.6.d-2	RHOMBOHEDRAL UNIT CELLS FILL SPACE	109
III.3.a-1	TWO-DIMENSIONAL SQUARE LATTICE	138

III.4.a-1	STAIRCASE OF STEPS FORMING A SCREW	143
III.4.a-2	SYMMORPHIC AND 2_1 SCREWS	143
III.4.a.ii-1	CRYSTALLOGRAPHIC SCREW ANGLES ARE LIMITED	146
III.4.b-1	GLIDE PLANE	147
III.4.f-1	CRYSTAL WITH A NONSYMMORPHIC GROUP . . .	156
III.4.f-2	A SQUARE CRYSTAL WITH A NONSYMMORPHIC GROUP	156
III.5-1	UNIT CELL OF DIAMOND	160
III.5-2	DIAMOND GLIDE PLANE AND SCREW AXIS	162
III.8.a-1	ONE-DIMENSIONAL "CRYSTALS"	173
III.8.a-2	THE FRIEZE GROUPS	174
IV.2.c.iv-1	RECTANGULAR-LATTICE BRILLOUIN ZONE	192
IV.2.c.iv-2	HEXAGONAL-LATTICE BRILLOUIN ZONE	192
IV.2.c.iv-3	BRILLOUIN ZONE OF CENTERED RECTANGLE . . .	193
IV.3.a-1	WIGNER-SEITZ CELL OF CENTERED RECTANGLE .	198
IV.3.e-1	THE RHOMBIC DODECAHEDRON	202
IV.3.e-2	ELONGATED DODECAHEDRON	202
IV.3.e-3	TRUNCATED OCTAHEDRON	203
IV.3.g.i-1	PROJECTION OF A HEXAGONAL PRISM	204
IV.3.g.iii-1	FACES OF A TETRAHEDRON DO NOT FORM BANDS	207
IV.3.g.iii-2	BANDS FOR THE ELONGATED DODECAHEDRON .	207
IV.3.g.v-1	NEAREST NEIGHBORS FOR BODY-CENTERED CUBE	208
IV.3.g.v-2	THE FACE-CENTERED CUBIC LATTICE	209
IV.5.a.ii-1	THE WIGNER-SEITZ CELL OF THE FCC LATTICE .	217
IV.5.a.ii-2	TWO VIEWS OF THE WIGNER-SEITZ CELL	217
IV.5.a.iii-1	BODY-CENTERED SQUARE LATTICE	218
IV.5.a.iii-2	BODY-CENTERED CUBIC LATTICE AND VECTORS	219
IV.5.a.iii-3	BODY-CENTERED CUBE AND WIGNER-SEITZ CELL	219
IV.5.a.iii-4	CONSTRUCTION OF TRUNCATED OCTAHEDRON	220
IV.5.b.i-1	WIGNER-SEITZ CELL OF TETRAGONAL LATTICE .	222
IV.5.b.i-2	THE BASE-CENTERED TETRAGONAL IS PRIMITIVE	222
IV.5.b.ii-1	STRETCHED WIGNER-SEITZ CELL IS NOT ONE . . .	223
IV.5.b.iii-1	BODY-CENTERED TETRAGONAL LATTICE	224
IV.5.b.iv-1	REPLACING THE FACE-CENTERED LATTICE	224
IV.5.b.v-1	SHRINKING A FACE-CENTERED CUBE	225
IV.5.b.v-2	ELONGATED DODECAHEDRON FOR THE LATTICE	225
IV.5.b.v-3	TOP VIEW OF LATTICE AND WIGNER-SEITZ CELL .	225
IV.5.b.vi-1	THE TETRAGONAL LATTICE THAT IS CUBIC . . .	227
IV.5.b.vii-1	CHANGE OF WIGNER-SEITZ CELL TYPE	228
IV.5.b.vii-2	WIGNER-SEITZ CELL CHANGING TYPE	229
IV.5.e-1	THE HEXAGONAL PRISM CANNOT BE DISTORTED	236
IV.6.a.i-1	BRILLOUIN ZONE OF THE SIMPLE CUBIC LATTICE	241

IV.6.a.ii-1	BRILLOUIN ZONE OF BCC LATTICE	241
IV.6.a.ii-2	BCC BRILLOUIN ZONE WITH LABELS	242
IV.6.a.iii-1	BRILLOUIN ZONE OF THE FCC LATTICE	243
IV.6.b-1	PRIMITIVE-TETRAGONAL BRILLOUIN ZONE	243
IV.6.b-2	STRETCHING DOES NOT GIVE A PROPER CELL	244
IV.6.b-3	FIRST BRILLOUIN ZONE FOR THE TETRAGONAL-I	245
IV.6.b-4	SECOND TETRAGONAL-I BRILLOUIN ZONE	245
VII.6.b-1	SPECIAL AND GENERAL VECTORS OF THE SQUARE	373
VII.6.c-1	STARS OF GENERAL VECTORS OF THE SQUARE?	373
VII.6.c-2	STAR FOR A SPECIAL POSITION	374
VII.6.c-3	VECTOR TO THE MIDPOINT OF BOUNDARY	375
VII.6.d-1	RECTANGLE WITH GENERAL AND SPECIAL POINTS	376
VII.6.h-1	UNIT CELL WITH GLIDES	380
VIII.4.e-1	COLORS SQUARE	422
VIII.4.f-1	ANTIFERROMAGNETIC ORTHORHOMBIC CELL	425
X.2.d-1	LINEAR TRIATOMIC MOLECULE	518
X.5.a-1	WATER MOLECULE	530
X.5.a.ii-1	A_1 MODE OF WATER	534
X.5.a.ii-2	A_1' MODE OF WATER	535
X.5.a.ii-3	B_2 MODE OF WATER	535
X.5.b-1	AMMONIA	537
X.5.b.ii-1	AMMONIA MODES WITH NONVIBRATING N	540
X.5.b.ii-2	AMMONIA MODES WITH MOVING NITROGEN	540
X.5.c-1	TETRAARSENE AND METHANE	545
X.5.c-2	BENZENE AND ETHYLENE	545
XI.2.j.i-1	NONSymmorphic HEXAGONAL UNIT CELL	591
XI.2.j.i-2	TRANSLATION IN THIS NONSYMMORPHIC CELL	591
XI.2.j.i-3	GLIDE IN THIS NONSYMMORPHIC CELL	592
XI.2.j.i-4	MIRRORS IN NONSYMMORPHIC HEXAGONAL CELL	592
XI.2.j.ii-1	BRILLOUIN ZONE FOR HEXAGONAL LATTICE	593
C-1	THE CUBE, WITH SYMMETRY GROUP O_h	637
C-2	BREAKING THE SYMMETRY TO O	638
C-3	A QUESTION MARK DESTROYS INVERSION SYMMETRY	638
C-4	CUBE WITH COMMA BREAKING INVERSION SYMMETRY	639
C-5	A TETRAHEDRON IN A CUBE	639
C-6	OBJECT INVARIANT UNDER T_d	640
C-7	INVARIANCE OF THE TETRAHEDRON	640

C-8	OBJECTS INVARIANT UNDER T_h	641
C-9	TETRAHEDRON WITH SYMMETRY GROUP T . . .	642
C-10	A CUBE WITH COMMAS INVARIANT UNDER D_4 .	642
C-11	D_4 IS NONABELIAN	643
C-12	OBJECTS INVARIANT UNDER D_{4h} AND C_{4h} . . .	643
C-13	OBJECTS INVARIANT UNDER D_4 AND D_{4h}	644
C-14	TRANSFORMATIONS OF OBJECT INVARIANT UNDER D_4	644
C-15	D_{2d} AND S_4 SYMMETRY	645
C-16	EXAMPLE OF SYMMETRY GROUP C_{4v}	645
C-17	SYMMETRY UNDER D_{6h} AND SUBGROUPS	646
C-18	THE SYMMETRIES OF C_{3h} AND SUBGROUPS . . .	646
C-19	OBJECT INVARIANT UNDER C_{3h}	647
C-20	OBJECTS INVARIANT UNDER C_{6h} AND C_{6v} . . .	647
C-21	OBJECTS INVARIANT UNDER D_3 AND C_{3v}	647
C-22	OBJECTS INVARIANT UNDER D_{3h} , D_{3d} AND S_6 .	648
C-23	THE EFFECT OF C_{2h} , C_{2v} AND S_2	648
C-24	THE ACTION OF D_{2h} AND SUBGROUPS	649
D-1	SYMBOLS AND MOTIF FOR WALLPAPER GROUPS	650
D-2	WALLPAPER GROUP $p1$ ($p1$)	650
D-3	WALLPAPER GROUP $p2$ ($p211$)	651
D-4	WALLPAPER GROUP pm ($p1m1$)	651
D-5	WALLPAPER GROUP pg ($p1g1$)	651
D-6	WALLPAPER GROUP cm ($c1m1$)	651
D-7	WALLPAPER GROUP pmm ($p2mm$)	652
D-8	WALLPAPER GROUP pmg ($p2mg$)	652
D-9	WALLPAPER GROUP pgg ($p2gg$)	652
D-10	WALLPAPER GROUP cmm ($c2mm$)	652
D-11	WALLPAPER GROUP $p4$ ($p4$)	653
D-12	WALLPAPER GROUP $p4m$ ($p4mm$)	653
D-13	WALLPAPER GROUP $p4g$ ($p4gm$)	653
D-14	WALLPAPER GROUP $p3$ ($p3$)	653
D-15	WALLPAPER GROUP $p3m1$ ($p3m1$)	654
D-16	WALLPAPER GROUP $p31m$ ($p31m$)	654
D-17	WALLPAPER GROUP $p6$ ($p6$)	654
D-18	WALLPAPER GROUP $p6m$ ($p6mm$)	654