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 rotation group 8

I.4.b The finite subgroups for three-dimensions 8

I.4.c Regular polyhedra 10

I.4.c.i *Determination of the regular polyhedra* . 10

I.4.c.ii *Other ways of determining these polyhedra* 13

I.4.c.iii *Dual polyhedra* 15

I.4.c.iv *Extensions and generalizations* 16

I.4.d How the rotation group determines its finite subgroups 17

I.4.d.i *Orbits and poles and why there are different types* 17

I.4.d.ii *The number of orbits and the finite subgroups* 19

I.4.d.iii *Implications and extensions* 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 *Naming the point symmetry transformations* 28
I.6.a.ii *The point symmetry transformations* . . . 29
I.6.a.iii *Why only some transformations are considered* 33
I.6.b Naming and describing the point groups 33
I.6.b.i *Point groups with only rotations* 35
I.6.b.ii *Restrictions on orders of point groups from their characters* 36
I.6.c Point groups with reflections 39
I.6.c.i *Cyclic groups with reflections* 39
I.6.c.ii *Dihedral groups with reflections* 40
I.6.c.iii *Adding reflections to the groups of regular polyhedra* 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 *Dihedral groups* 52
I.7.a.ii *Cubic groups* 52
I.7.a.iii *The structure of improper point groups* . . 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 *Conditions given by two-dimensional lattices* 98
II.5.a.ii *The points allowed by the two-dimensional sublattices* 99
II.5.a.iii *Adding points simultaneously* 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 *The monoclinic lattices* 113
II.7.b.ii *Tetragonal lattices* 114
II.7.b.iii *The orthorhombic lattices* 116
II.7.b.iv *The trigonal and hexagonal lattices* 118

II.7.b.v *The cubic system* 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 *The space group with a screw and the point group* 144
III.4.a.ii *Limitations on crystallographic screws* . . 145
III.4.a.iii *Pairs of enantiomorphic screws* 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 *These are the — only — nonprimitive operations* 149
III.4.c.ii *Nonprimitive operations are determined by primitive ones* 151
III.4.d The factor group of a space group gives a point group 152
III.4.d.i *Cosets and coset representatives* 153

III.4.d.ii *The difference in factor groups of symmorphic and nonsymmorphic groups* . . . 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 *How the crystal differs from the lattice* . . 157
III.4.f.ii *The space group operations* 157
III.4.f.iii *Shifting the origin cannot make the group symmorphic* 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 *Placing glides* 164
III.5.b.ii *Placing screws* 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 NONSYMMORPHIC GROUPS 167
III.6.a Are nonsymmorphic space groups semi-direct products? 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 *Description of the two-dimensional space groups* 176
III.8.b.ii *Notation and illustrations for the wallpaper groups* 178
III.9 THE THREE-DIMENSIONAL SPACE GROUPS 180
III.9.a The symmorphic space groups 180
III.9.a.i *Ambiguities of setting give more space groups* 181
III.9.a.ii *Why are these the symmorphic space groups?* 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 *Brillouin zones are of the lattice* 190
IV.2.c.ii *Symmetry of points in the Brillouin zone* . 190
IV.2.c.iii *Boundaries of Brillouin zones* 191
IV.2.c.iv *Examples of two-dimensional Brillouin zones* 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 *The two-dimensional projections of the cells* 204
IV.3.g.ii *The cells are centrosymmetric* 205
IV.3.g.iii *The faces form bands* 205
IV.3.g.iv *Sharing by adjacent cells* 207
IV.3.g.v *Counting nearest neighbors* 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 *The simple cube* 216
IV.5.a.ii *The face-centered cubic lattice* 216
IV.5.a.iii *The body-centered cubic lattice* 218
IV.5.b The tetragonal system 221
IV.5.b.i *The primitive tetragonal lattice* 221
IV.5.b.ii *The tetragonal Wigner-Seitz cell is not a stretched cubic Wigner-Seitz cell* 222
IV.5.b.iii *The body-centered tetragonal lattice* . . . 223
IV.5.b.iv *The all-face-centered lattice* 224

IV.5.b.v *Why the tetragonal has fewer lattices than the cubic* 224
IV.5.b.vi *The differing Wigner-Seitz cells of the lattice* 226
IV.5.b.vii *How cells change* 227
IV.5.b.viii *Surfaces appear when edges disappear* . 229
IV.5.b.ix *Cells as limits of others* 230
IV.5.c The orthorhombic system 230
IV.5.c.i *The simple orthorhombic lattice* 231
IV.5.c.ii *The two-face-centered orthorhombic lattice* 231
IV.5.c.iii *The all-face-centered orthorhombic lattice* 232
IV.5.c.iv *The body-centered orthorhombic lattice* . 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 *The Brillouin zone of the simple cube* . . . 240
IV.6.a.ii *The Brillouin zone of the body-centered cubic lattice* 241
IV.6.a.iii *The Brillouin zone of the face-centered cubic lattice* 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 cylic 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 *The multiplicator* 262
V.4.b.ii *The Abelian group formed by the factor classes* 262
V.4.b.iii *All factors give projective representations* 263
V.4.b.iv *The factors are roots of unity* 265
V.4.b.v *Properties of factor systems and projective representations* 266
V.4.c Some groups with projective representations . . . 267
V.4.c.i *Projective representation of cyclic groups and products* 267
V.4.c.ii *Dihedral groups* 269
V.5 CENTRAL EXTENSIONS 270
V.5.a Nonuniqueness of central extensions 271
V.5.a.i *Symmetric group S_3 as a central extension* 271
V.5.a.ii *Why central extensions are not unique* . . 272
V.5.a.iii *Central extension of the four-group* 272
V.5.b Central extensions and factor systems 274
V.5.b.i *The multiplicator and central extensions* . 276
V.5.b.ii *The meaning of projective representation* 276
V.5.b.iii *The covering group* 277
V.5.b.iv *Why only one factor system is considered* . 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 normal subgroup 323
VI.7.c Allowable representations of the little group . . . 324
VI.7.d All representations are given by the allowable representations 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 *Translation representations are scalars in little groups* 348
VII.3.a.ii *Representations can be obtained from the little co-group* 349
VII.3.a.iii *The induced representation matrices* . . 350
VII.3.a.iv *The point group part of the matrices* . . 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 *These matrices form a representation* . . . 357
VII.4.c.ii *The representations are irreducible* 357
VII.4.c.iii *All inequivalent representations are obtained* 359
VII.4.d The allowable representations of the little group . 359
VII.4.d.i *Obtaining the allowable representations from representations of the little co-group* 359
VII.4.d.ii *The cases of internal vectors* 361
VII.4.d.iii *Special positions on the boundary* 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 *The little groups and the representations* 377
VII.6.f.ii *What determines the little groups?* 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 *The representation basis functions* 383
VII.6.i.ii *How the glide affects basis functions* . . . 384
VII.7 THE CUBIC AND DIAMOND STRUCTURES 384
VII.7.a The representations of the factors for $Fm3m$ . . . 389
VII.7.b The representations of the factors for $Fd3m$ . . . 389
VII.7.b.i *Representations at Point* Γ 390
VII.7.b.ii *Points with nonsymmorphic little groups* . 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 *Potentially real, and pseudo-real, representations* 405
VIII.3.c.ii *Ambivalent groups and their character sets* 406
VIII.3.c.iii *Why physically are groups so classified?* 407
VIII.3.c.iv *Reality and the rotation group* 409

VIII.3.d Equivalent sets can be distinguishable 410
VIII.3.d.i *Mathematical equivalence, and physical equivalence* 411
VIII.3.d.ii *Complexity of half-integral angular momentum statefunctions* 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 *Cyclic color groups* 415
VIII.4.b.ii *Dihedral color groups* 416
VIII.4.b.iii *Gray groups* 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 *The square has other magnetic groups* . 422
VIII.4.e.ii *Why the square has these magnetic groups* 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 *Transforming to reduced form* 444
VIII.7.i.ii *The case with the sign positive* 446
VIII.7.i.iii *The case with the minus sign* 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 *The procedure for unitary groups* 457
VIII.9.b.ii *How the procedure is changed for magnetic space groups* 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 *Unitary magnetic little groups* 462
VIII.9.d.ii *Magnetic little groups with antiunitary operators* 463
VIII.9.d.iii *Degeneracies depend on the magnetic corepresentation* 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 *Tensors formed from products of vectors* . 473
IX.2.b.ii *Restrictions on crystal properties* 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 properties 477
IX.3.a.i *Neumann's principle* 477
IX.3.a.ii *Is Neumann's principle obvious?* 478
IX.3.a.iii *Why tensor components are point-group scalars* 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 *The meaning of the symmetric and antisymmetric parts* 490
IX.5.a.ii *The physical quantities given by the symmetric parts* 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 *Kinetic energy, potential energy and normal coordinates* 523
X.3.a.ii *Proof of the existence of normal coordinates* 525
X.3.b Finding normal coordinates 526
X.3.b.i *Valence bond lengths and interbond angles* 527
X.3.b.ii *Coordinates that are not independent* . . . 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 *The vibrational representations* 531
X.5.a.ii *The symmetry coordinates* 533
X.5.a.iii *Internal coordinates for water* 536
X.5.b Ammonia 537
X.5.b.i *The vibrational representations* 538
X.5.b.ii *Displacements in the normal modes* 539
X.5.b.iii *The two-dimensional E modes* 541
X.5.b.iv *Internal coordinates for ammonia* 542
X.5.b.v *Why is group theory relevant here?* 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 *Raman scattering is of second order* 556
X.7.b.ii *The angular-momentum selection rules* . . 557
X.7.b.iii *Exclusion rule* 558
X.7.b.iv *Raman scattering for crystals* 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 *Point groups differ at different points in reciprocal space* 572
XI.2.c.ii *How these bands illustrate the meaning of space group representations* 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 *The simple cubic lattice* 579
XI.2.h.ii *The body-centered cubic lattice* 584
XI.2.h.iii *The face-centered cubic lattice* 585
XI.2.i Energy bands for nonsymmorphic groups 586
XI.2.i.i *Sticking together of bands* 586
XI.2.i.ii *Irreducible representations on the zone faces* 587
XI.2.i.iii *The little group need not be a subgroup of the point group* 589
XI.2.j The close-packed hexagonal structure 590
XI.2.j.i *Nonsymmorphic elements of the crystal* . 590
XI.2.j.ii *Special positions of the Brillouin zone* . . . 592
XI.2.j.iii *Representations, and the effect of nonsymmorphic elements* 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 *Some different possibilities* 602
XI.5.a.ii *Steps in the decomposition* 602
XI.5.b The octahedral group as an example 603
XI.5.b.i *The intermediate case* 603
XI.5.b.ii *The case of a weak crystal field* 605
XI.5.b.iii *Splitting of the octahedral levels* 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 *Tetrahedral carbon* 611
XI.7.d.ii *Trigonal carbon* 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 *Magnetic ordering* 618
XI.8.f.ii *Alloys* 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 *The third-order term must be zero* 625
XI.8.k.ii *The fourth-order term* 626
XI.8.k.iii *The requirement of spatial homogeneity* . 626
XI.8.l Halving the symmetry always allows a transition . 627
XI.8.m Active and passive representations 627

XI.9 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