

Contents

<i>Preface</i>	<i>page</i> xi
<i>Notation and conventions</i>	xiii
1 The elementary properties of groups	1
1.1 Definitions	1
1.2 Conjugate elements and classes	5
1.3 Subgroups and cosets	6
1.4 The factor group	8
1.5 Minimal content of Sections 1.6, 1.7, and 1.8	12
1.6 Product groups	15
1.7 Mappings, homomorphisms, and extensions	17
1.8 More about subgroups and classes	18
Problems	22
2 Symmetry operators and point groups	23
2.1 Definitions	23
2.2 The multiplication table – an example	32
2.3 The symmetry point groups	36
2.4 Identification of molecular point groups	48
Problems	50
3 Matrix representatives	53
3.1 Linear vector spaces	53
3.2 Matrix representatives of operators	55
3.3 Mappings	60
3.4 Group representations	62
3.5 Transformation of functions	62
3.6 Some quantum mechanical considerations	67
Problems	68
4 Group representations	70
4.1 Matrix representations	70
4.2 Irreducible representations	72
4.3 The orthogonality theorem	73
4.4 The characters of a representation	74
4.5 Character tables	80
4.6 Axial vectors	82

viii Contents

4.7	Cyclic groups	86
4.8	Induced representations	88
	Problems	95
5	Bases of representations	96
5.1	Basis functions	96
5.2	Construction of basis functions	97
5.3	Direct product representations	99
5.4	Matrix elements	101
	Problems	105
6	Molecular orbitals	106
6.1	Hybridization	106
6.2	π Electron systems	109
6.3	Equivalent bond orbitals	114
6.4	Transition metal complexes	117
	Problems	129
7	Crystal-field theory	131
7.1	Electron spin	131
7.2	Spherical symmetry	132
7.3	Intermediate crystal field	134
7.4	Strong crystal fields	139
	Problems	146
8	Double groups	148
8.1	Spin-orbit coupling and double groups	148
8.2	Weak crystal fields	152
	Problems	154
9	Molecular vibrations	156
9.1	Classification of normal modes	156
9.2	Allowed transitions	158
9.3	Inelastic Raman scattering	161
9.4	Determination of the normal modes	162
	Problems	168
10	Transitions between electronic states	171
10.1	Selection rules	171
10.2	Vibronic coupling	173
10.3	Charge transfer	178
	Problems	181
11	Continuous groups	182
11.1	Rotations in \mathfrak{R}^2	182
11.2	The infinitesimal generator for SO(2)	183
11.3	Rotations in \mathfrak{R}^3	184
11.4	The commutation relations	187
11.5	The irreducible representations of SO(3)	192

 Contents

ix

11.6	The special unitary group $SU(2)$	200
11.7	Euler parameterization of a rotation	205
11.8	The homomorphism of $SU(2)$ and $SO(3)$	208
	Problems	216
12	Projective representations	218
12.1	Complex numbers	218
12.2	Quaternions	220
12.3	Geometry of rotations	222
12.4	The theory of turns	225
12.5	The algebra of turns	228
12.6	Projective representations	232
12.7	Improper groups	240
12.8	The irreducible representations	243
	Problems	250
13	Time-reversal symmetry	252
13.1	Time evolution	252
13.2	Time reversal with neglect of electron spin	253
13.3	Time reversal with spin–orbit coupling	254
13.4	Co-representations	257
	Problems	264
14	Magnetic point groups	265
14.1	Crystallographic magnetic point groups	265
14.2	Co-representations of magnetic point groups	267
14.3	Clebsch–Gordan coefficients	277
14.4	Crystal-field theory for magnetic crystals	280
	Problems	281
15	Physical properties of crystals	282
15.1	Tensors	282
15.2	Crystal symmetry: the direct method	286
15.3	Group theory and physical properties of crystals	288
15.4	Applications	293
15.5	Properties of crystals with magnetic point groups	303
	Problems	305
16	Space groups	307
16.1	Translational symmetry	307
16.2	The space group of a crystal	314
16.3	Reciprocal lattice and Brillouin zones	324
16.4	Space-group representations	331
16.5	The covering group	336
16.6	The irreducible representations of G	337
16.7	Herring method for non-symmorphic space groups	344
16.8	Spinor representations of space groups	351
	Problems	355

x Contents

17	Electronic energy states in crystals	357
17.1	Translational symmetry	357
17.2	Time-reversal symmetry	357
17.3	Translational symmetry in the reciprocal lattice representation	358
17.4	Point group symmetry	359
17.5	Energy bands in the free-electron approximation: symmorphic space groups	365
17.6	Free-electron states for crystals with non-symmorphic space groups	378
17.7	Spinor representations	383
17.8	Transitions between electronic states	384
	Problems	390
18	Vibration of atoms in crystals	391
18.1	Equations of motion	391
18.2	Space-group symmetry	394
18.3	Symmetry of the dynamical matrix	398
18.4	Symmetry coordinates	401
18.5	Time-reversal symmetry	404
18.6	An example: silicon	406
	Problems	412
	Appendices	
A1	Determinants and matrices	413
A2	Class algebra	434
A3	Character tables for point groups	447
A4	Correlation tables	467
	<i>References</i>	476
	<i>Index</i>	481