CAMBRIDGE

Cambridge University Press
978-0-521-64250-7 — Group Theory with Applications in Chemical Physics
Patrick Jacobs
Index
More Information

Index

Abelian group 2
acoustic mode 393
active representation 23
adiabatic potential 173
adjoint 54
  of an operator 102
adjoint matrix 418
algebra of turns 228
ambivalent class 435
angular momentum 184, 189
anharmonicity 160
  constant of 160
antibonding orbitals 106, 125
antiferromagnetic crystal 265
antilinear operator 252
antipole 223
antisymmetrical direct product 100
antisymmetrizing operator 141
antiunitary operator 252, 267, 405
associated Legendre functions 194
associative 2, 220
axial groups 82
axial tensor 283
axial vector 82

basic domain 331
basis 53, 96
  of a lattice 308
basis functions, construction of 97
bcc see body-centred cubic
benzene 104, 109, 174
Bethe 80, 150, 151
bilateral binary (BB) 232
binary composition 1, 15, 70
binary rotation 25
Bloch functions 317, 357
block-diagonal structure 404
body-centred cubic (*bcc*) 309
bonding orbitals 106, 125
Born and von Kármán boundary conditions 316
Born–Oppenheimer approximation 173
bra 102
Bragg reflection 358
Bravais lattice 311, 318
Brillouin zone 327, 329, 358, 397
BSW notation 361, 362, 370

c-tensors 303
Cartan gauge 204, 210, 240, 241, 242
Cartesian tensors 360
Cayley–Klein parameters 202, 243, 351
celebrated theorem 79
central extension 336, 337, 367
centralizer 14, 19, 434
centre 19
character 74, 99
character system 74
character tables 76–78, 80, 447
character vector 259
characteristic equation 420, 441
charge overlap 107
charge transfer 178
chemical bond 106
class 5, 19
class algebra 439
class constants 436
class property 440
Clebsch–Gordan series 209, 277, 385
closed shell 172
closo $B_n H_n^{-2}$ 51
closure 1, 393
co-factor 413
coincidence 162
column matrix 415
combination bands 160
commutation relations (CRs) 131, 187
compatibility relations 362
complementary IR 303
complementary minor 413
complementary operators 265
complex conjugate 218
complex conjugation operator 253
complex number 218
complex plane 219
complex quaternion parameters 244
component (of a vector) 57
Condon and Shortley (CS) choice of phase 190
conical transformation 195
conjugate 18
conjugate bases 292
conjugate elements 5
continuous groups 182
conventional unit cells 309
co-representation 257, 267, 269–273
correlation tables 467
corresponding elements 43
coset 7
  expansion 318
  representatives 7
coupled representation 210
covering group 336, 337
crystal classes 311
crystal field
  intermediate 134

© in this web service Cambridge University Press www.cambridge.org

CAMBRIDGE

Cambridge University Press
978-0-521-64250-7 — Group Theory with Applications in Chemical Physics
Patrick Jacobs
Index
More Information

crystal field (cont.)
  strong 139
  weak 152
crystal pattern 307
crystallographic orbit 321
crystallographic point groups 45, 46, 310
crystals (physical properties of) 282
cubic groups 244
cyclic group 3, 36, 86, 243
cyclobutadiene 130

degeneracy index 290
degenerate mode 161
delocalization energy 113
descending symmetry 140
determinants 413
diagonal matrix 420
diagonalization of the Dirac characters 440
diamond 378
dibenzene chromium 50
dihedral groups 36
dihedral planes 39, 41
dimension (of a representation) 70, 74
dimensionality (of a vector space) 53
dipole moment operator 159
Dirac character 14, 20, 434
Dirac notation 101, 102, 132
direct product
  of groups 8, 12, 39
  of matrices 99, 432
  of representations 99
  of sets 99
direct sum 72, 424
dispersion relation 393, 394
displacement vector 163
displacement vector space 162
double cosets 385
double group 82, 148, 149, 195, 248
dynamical matrix 392, 398

E_1 (electric dipole) transition 104, 171
E_2 (electric quadrupole) transition 104, 171
eigenvalues 393, 420
eigenvector 97, 99, 420
Einstein summation convention 186, 282
elastic constants (third order) 296
elastic stiffness 286
electrical conductivity 298
electrochemical potential 297
electron spin 131
empty lattice approximation 366
energy bands 357, 360, 371
entropy production 288
equivalent matrices 420
equivalent points 327
equivalent positions 320
equivalent representations 72, 259
equivalent wave vector 331
Euler angles 205
Euler construction 223
Euler–Rodrigues parameters 230
Euler's formula 219
extended zone 359
extension 320

face-centred cubic (*fcc*) 308
factor group 8, 12, 319, 407
factor system 234
faithful representation 58
ferrimagnetic crystal 265
ferrocene 50
ferromagnetic crystal 265
ferromagnetism 304
fcc see face-centred cubic
fibre 13
fine structure constant 133, 173
flux 288
force constants 391
free-electron approximation 357, 366
frequency 92, 385
Frobenius reciprocity theorem 93
Frobenius–Schur test 261, 273, 405
function operator 63, 183, 316
function space 97, 104
fundamental theorem (Nowick) 290
fundamental theorem (Onsager) 288
fundamental transition 159
fundamental translations 307

galvanomagnetic effects 299
geometry of rotations 222
germanium 378, 406
glide plane 318
ground representation 88
group 1
  of the Hamiltonian 68, 96
  of the Schrödinger equation 68
  of the wave vector 367
group generators 3
group representation 62
gyration tensor 294

Hall tensor 302
halving subgroup 265
Hamiltonian 133
  invariant under R 67
harmonic approximation 160, 391
Hermitian matrix 421
Hermitian scalar product 54
Herring factor group 344
Herring group 344, 367
Herring multiplication rule 345
Herring's method 335, 344
holosymmetric space group 331
homomorphism 208
homomorphous group 14
Hückel 113
Hund's rules 134, 144
hybridization 106, 116

i-tensors 303
icosahedral point group 37, 244
identity 2, 28, 223
identity representation 70
image 13, 60
indicatrix 284

© in this web service Cambridge University Press www.cambridge.org

CAMBRIDGE

Cambridge University Press
978-0-521-64250-7 — Group Theory with Applications in Chemical Physics
Patrick Jacobs
Index
More Information

induced representation 90
improper axis 28
improper rotation 26, 282
indices 7, 309
indistinguishability 3
indium antimonide 384
induced representation 88, 93
infinitesimal generator 183, 189
infinitesimal rotation 83, 284
inner direct product 16
integral invariance 196
International notation 28, 36, 267
intertwining matrix 427
intertwining number 93
invariant subgroup 7, 8
inverse 2
inverse class 22, 434
inversion operator 58
irreducibility criterion 92
irreducible representation (IR) 73, 243
irreducible volume 397
irregular operations 233, 243
irreversible processes 288
isomorphous group 2, 42

Jahn–Teller effect 175
Jones symbol 58

kernel 17, 336
Kerr effect 296
ket 102
Kramers' theorem 151, 256

LA mode 409
LO mode 410
Lagrange's theorem 21
Lagrangian strain 296
Laporte rule 171
LCAO approximation 109
left coset 88
length (of a vector) 55
Levi–Civita three-index symbol 185
linear operator 252
linear response 288
linear vector space 53
little co-group 327, 333
little factor group 332
little group 332, 367
lowering operator 132

M_1 (magnetic dipole) transition 104, 171
magnetic point groups 265, 303
  crystal-field theory for 280
magnetoelectric polarizability 304
many-electron atom 133
mapping 13, 60
matrices 415
  special 418, 420
matrix element 102, 103
matrix multiplication 415
matrix representation 53, 70, 424
matrix representative 56, 57, 415
metric 55, 311
Miller indices 309, 328
mixing coefficient 115
modulus 219
molecular orbital 107, 115
molecular point groups 48
Morse potential 160
Mulliken 81
Mulliken–Herzberg notation 151
multiplet 133
multiplication table 1, 34
multiplier representation 400

negative hemisphere 223
negative rotation 24
Nernst tensor 301
Neumann's principle 282, 288
non-symmorphic space group 318, 344, 367, 378
norm 221
normal matrix 420
normal mode coordinates 156, 162, 163, 164
normal modes 156
  symmetry of 156
normalization 112
normalized basis 285
normalized vector 55
normalizer 19

O(3) 203, 208, 240
occupation number representation 159
octahedral complex 117, 174
octahedral point group 37
Onsager 288
Onsager reciprocal relations (ORR) 288, 298
Opechowski's rules 149
optic mode 393
optical activity 294
optical energies 178
orbital approximation 133
order
  of a class 5, 21
  of a group 2
  of an axis 23
orthogonal group O(3) *see* O(3)
orthogonal matrix 61, 421
orthogonality theorem 73, 425, 428, 430
  for the characters 76, 77, 195
orthonormal basis 55
orthonormal eigenvectors 393
outer direct product 15
overlap integral 112
overtone 161

π bond 106, 126
π electron systems 109, 113
parity 136, 164, 167, 209
parity selection rule 171, 174
passive representation 23
Pauli exclusion principle 133, 140
Pauli gauge 204, 211, 240, 242, 243
Pauli matrices 200
Pauli repulsion 145
Peltier effect 298
pentagonal dodecahedron 37

© in this web service Cambridge University Press www.cambridge.org

CAMBRIDGE

Cambridge University Press
978-0-521-64250-7 — Group Theory with Applications in Chemical Physics
Patrick Jacobs
Index
More Information

periodic boundary conditions (PBCs) 316, 326, 357, 366, 397
periodicity (of the reciprocal lattice) 394
permutation 3
permutation matrix 88, 419
permutation representation 372, 375
phase factor 67
phenomenological coefficients 288
  relations 288
piezomagnetic effect 305
plane waves 392
Pockels effect 296
point group 30, 48
  of a space group 318
  of the wave vector 327, 332, 360, 407
point group generators 286
point subgroup 317
point symmetry operations 28
polar vector 26
polarizability 161
pole (of a rotation) 222
pole conventions 245
poles (choice of) 223
positive hemisphere 222
positive rotation 24
primitive lattice 308
principal axis transformation 284
principal minor 423
projection (of a vector) 56
projection diagram 27
projection operator 98, 366, 368, 403, 408
projective factor 233, 274
projective representation 67, 195, 218, 233, 234, 333, 335, 400
prongs (of a star) 385, 386
proper point group 36
proper rotations 282
properties of the characters 74
pseudoscalar 26, 211, 282
pseudovector 26, 82, 220

quaternion 220
quaternion conjugate 221
quaternion group 226, 443
quaternion parameters 230, 351
quaternion units 220

raising operator 132
Raman scattering 161
range (of ϕ) 23
rearrangement theorem 1
reciprocal lattice 324
reduced zone 359
reduction (of a representation) 78
reflection 59
regular classes 233, 384
regular operation 233
regular representation 79
repeat index 290
representation domain 332
required representations 345, 346
right-handed axes 23
Rodrigues 225
rotation 23
rotation operator 23
rotation parameter 223
rotational motion 156
rotational symmetry 310
rotations
  in $\Re^2$ 182
  in $\Re^3$ 184
rotoreflection axis 28
rotoreflection operator 27
row matrix 415
Russell–Saunders coupling 132, 133
Russell–Saunders multiplets 148, 152

σ bond 106
sc see simple cubic lattice
scalar 209, 282
scalar product 101, 102
Schmidt orthogonalization 112
Schönflies notation 28, 80, 267
Schur's lemma 259, 270, 291, 425, 426
screw rotation 318
Seebeck effect 298
Seitz operator 314
semidirect product 13
setting 322
shell model 411
shift operators 188
Shubnikov 265
silicon 378, 384, 406
similarity of orientation 289
similarity transformation 72, 416, 420
simple cubic (*sc*) lattice 368
singlet state 141
singular matrix 416
site symmetry 321
space group 314
space group representations 331, 336, 339
space group symmetry 394
space lattice 307
special orthogonal groups
  SO(2) 182, 184
  SO(3) 61, 182, 184, 192, 203, 208, 231
special orthogonal (SO) matrices 61
special unitary groups
  SU(2) 200, 202, 208
  SU′(2) 203
spectral term 133
spherical harmonics 193
spherical vector 194
spin eigenvector 132, 133
spin–orbit coupling 104, 133, 148, 173, 281
spin orbital 103
spin pairing 145
spin postulate 131
spin quantum number 131
spin selection rule 103, 171
spinor 209
spinor representation 82, 149, 232, 236, 237
standard parameters 235
standard representation 246
standardization 240
star 332, 333

© in this web service Cambridge University Press www.cambridge.org

CAMBRIDGE

Cambridge University Press
978-0-521-64250-7 — Group Theory with Applications in Chemical Physics
Patrick Jacobs
Index
More Information

stereographic projection 213
Stern–Gerlach experiment 131
subduced representation 93
subduction 93, 138, 223
subgroup 6
sum rule 391
symmetric group 4, 5
symmetric tensor 284
symmetrical direct product 100
symmetrizing operator 141
symmetry coordinates 289, 401, 403
symmetry element 27, 28
symmetry groups
  lower 294
  upper 294
symmetry operations 23, 26
symmorphic space group 318, 333, 367

TA mode 411
TO mode 411
tensor 209, 282
  of rank 2 209
  of rank *n* 283
tensor properties of crystals 282
tetrahedral point group 37
thermal conductivity 298
thermodynamic force 288
thermoelectric effects 297
thermoelectric power 298
thermomagnetic effects 299
time-evolution operator 253
time reversal 252, 255, 358, 404
time-reversal symmetry 262
total angular momentum 131, 148
totally symmetric representation 70
trace of a matrix 416
trans-dichloroethylene 50
transform 5, 21
transformation
  of functions 63, 64
  of operators 102
transition metal complexes 117
transition probability 104, 171, 388
translation subgroup 316
translational motion 156
translational symmetry 307, 357, 391
translations 27
transposed matrix 61
triplet state 141
turn 225

uniaxial groups 294
unimodular 201
unit cell 307–310, 325, 327
unitary basis 55
unitary matrix 61, 422
unitary operator 252
unitary representation 424
upper cubic groups 301

vector representations 81
vibrational motion 156
  degeneracy of 158
vibrational quantum number 159
vibronic coupling 104, 173
vibronic interaction 173, 175
Voigt notation 284, 286
von Laue conditions 358

wave vector 392
Wigner–Seitz cell 309, 327
Wyckoff position 321

zero overlap appproximation (ZOA) 112
zone boundary 368

© in this web service Cambridge University Press www.cambridge.org