

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

482 Index

- 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

- 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–Hertzberg 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

484 Index

- 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 \mathfrak{R}^2 182
 in \mathfrak{R}^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

- 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 approximation (ZOA) 112
 zone boundary 368