

# Index

- $\delta$  127  
 $\Delta$  224  
 $\Pi$  126  
 $\Pi$ -electron systems 263  
 $\sigma$  126  
 $\sigma_a$  mirror planes 193  
 $\sigma_h$  111  
 10Dq 224  
 3n-6 rule 81  
 Abelian 43, 110, 152, 153, 256, 349  
 active convention 84  
 ammonia 1, 173  
 angular momentum quantum number 281  
 angular momentum 281, 288  
 antisymmetric direct product 291  
 antisymmetric stretch vibration 79  
 ascent in symmetry 399  
 associative (multiplication) 346  
 atomic orbital model of ammonia 2  
 axes 102  
  
 banana bond 143  
 basis functions 42, 45, 360  
 black and white groups 349  
 body-centred cubic 310  
 bond stretch vibrations 76  
 Bravais lattice 308, 311  
 bridge hydrogens 136  
 Brillouin zones 327  
 bromine pentafluoride 145  
  
 $C_{4v}$  145  
 character table  $C_{2v}$  46,  $D_{2h}$  112,  $C_i$  116,  $D_2$  116,  $C_{3v}$  175,  $O$  192,  $C_{4v}$  146,  $O_h$  197,  $T_d$  249,  $I$  253,  $K$  255,  $C_4$  266  
 character 159, 359  
 character tables 40, 42, 369  
 $C_i$  115  
 class multiplication table 353  
 class (of operations) 349, 351  
 class algebra 352  
 class 147, 346  
 closed shells of electrons 292  
 closure 412, 346  
 complex conjugate 268, 270  
 complex characters 153  
 configuration 289  
 configuration interaction 293  
 conjugate elements 350  
 correlation tables 240, 241  
 crystal systems 299, 307  
 crystal field theory 218  
 crystallographic point groups 311  
  
 $D_2$  111  
 $D_{2h}$  111  
 degeneracy 145  
 diborane 136  
 dihedral 111  
 direct product 94, 114, 197, 238, 288, 334, 363  
 direct sum 208, 210  
 displacement vectors 81

424

double degeneracy 146, 159  
 double groups 282

electric dipole 100  
 electromagnetic radiation 99  
 electron deficiency 137  
 electron-repulsion model of ammonia 4  
 electron-spin 281  
 electron-spin-repulsion model of ammonia 6  
 element (of a group) 345  
 equivalent orbitals 144  
 ethene 109

face-centred cubic 310  
 factor group model 332, 333, 338

g (gerade) 117  
 glide planes 323  
 grey groups 349  
 group multiplication tables 36, 39  
 group 17, 345

Hermann-Mauguin notation 322, 407–409, 411–412  
 high spin 225  
 hybrid orbital model of ammonia 3

I 282  
 icosahedral symmetry 245  
 icosahedron 235  
 identity operation 16  
 improper symmetry operation 12, 15, 90  
 improper rotations 198  
 index (of a subgroup) 243  
 infrared spectroscopy 92  
 invariant subgroup 115, 236, 334  
 irreducible representations 40, 52

INDEX

isomorphism 100, 125, 141, 245  
 isomorphous groups 116, 347

jj limit 297

K(spherical group) 254

laboratory axes 102  
 lattice 299  
 law of combination 345  
 LCP (ligand close packing) 5  
 LGO (ligand group orbital) 210, 399–400  
 ligand 218  
 ligand field theory 225  
 linear molecules 261  
 localized orbitals 144  
 low spin 225

magnetic dipole 100  
 matrices 159  
 matrix algebra 355  
 matrix multiplication 356  
 Maxwell 99  
 mirror planes 15  
 moduli primitive translation 416–418, 421–422  
 molecular dynamics 238  
 molecular axes 102  
 Möbius strip 284  
 Mössbauer spectroscopy 336  
 multiplication 38, 345  
 multiplication table  $D_{2h}$  114,  $C_{3v}$  237, 347,  $C_{2v}$  39,  $C_4$  352  
 multipliers 19

nodal patterns  $D_2$  117,  $C_i$  119,  $C_{4v}$  160,  $O_h$  199,  $C_{2v}$  48,  $D_{2h}$  121,  $C_{3v}$  179,  ${}^2C_{2v}$  287  
 non-Abelian 153  
 non-crossing rule 279  
 non-invariant subgroups 238

- non-symmorphic space groups 322
- normal modes 103
- octahedral transition metal complexes 218
- operation 11
- optical activity 108, 297
- order (of a group) 46, 243
- order 153
- oriented gas model 333, 337
- orthonormality 45, 46, 98
- orthonormality theorems 146, 152
- pairing energy 225
- passive convention 84
- Pauli exclusion principle 292
- permutation groups 347
- point group allocation 232
- point group 17, 19
- polychromatic groups 349
- product functions 92, 288
- projection operators 109, 129, 131, 209, 290, 353
- proper rotations 198
- proper symmetry operation 12, 90
- pure rotational subgroup 244
- quantum mechanical integrals 96
- quasicrystals 251, 307
- R 282
- Raman spectroscopy 92
- reducible matrices 360
- reducible representations 51
- regular representation 270, 359
- relief of degeneracy 243
- representations 40
- rotation-inversion operations 251
- rotation-reflection operations 251
- Russell-Saunders coupling 297
- $S_2$  234
- $S_4$  operations 194
- $S_6$  operations 194
- Schmidt orthogonalization 247, 399
- Schönflies notation 407–409, 411–412
- screw axis 322
- selection rules 99
- separable degeneracy 152, 266
- Shubnikov groups 349
- single degeneracy 159
- site group model 333, 338
- space group 236
- spectroscopic selection rules 96
- spherical symmetry 245, 254
- spherical harmonics 260
- spin-orbit coupling 288
- spiropentane 233
- Stern-Gerlach 288
- strong field 225
- subgroup 236
- substitution groups 348
- symmetric group 347
- symmetric direct product 291
- symmetric stretch vibration 78
- symmetry operation 11
- symmetry adapted combinations 54, 129, 131, 164, 180, 210
- symmetry element 11, 19
- symmetry-enforced degeneracy 145
- symmorphic space groups 317
- term correlation diagram 279
- term 289, 291
- tetrahedral symmetry 245
- totally symmetric 41
- transformation as a pair 274
- translation vectors 300
- translational subgroup 308
- translational invariance 331
- translations 87
- triple direct products 101

426

triple degeneracy 193  
two-colour group 349

u (ungerade) 117  
unit cells 301, 325  
unit element 346  
unit cell model 332, 335

INDEX

VSER (valence shell electron  
repulsion) model 5, 145  
vibrational spectroscopy 75

Walsh diagram 68, 185  
weak field 225  
Wigner-Seitz unit cells 327