

Index

- ab initio calculations, 103, 384
 of magnetochiral birefringence, 330
 of optical rotation, 272–3, 304
 of Raman optical activity, 346
 of vibrational circular dichroism, 332, 340–2
 absolute configuration, 2–3
 of hexahelicene, 300–4
 of a two-group structure, 288–91
 absolute enantioselection, 23
 absorption, 5, 94–8, 134–5
 index, 5–8
 lineshape functions, 96, 105–6
 adamantanones
 magnetic circular dichroism, 326–7
 partition diagrams for, 256–8
 adiabatic approximation, 114–16
 crude, 120–1, 340, 389
 see also Born–Oppenheimer approximation;
 Herzberg–Teller approximation
 alkyl group perturbers, 296
 alternating (Levi–Civita) tensor, 179–81
 ammonia, inversion motion, 190–2
 angular frequency, 4, 56
 angular momentum
 of circularly polarized light, 409–11
 orbital, 70, 199–201; symmetry aspects, 29–30
 quantum states: matrix elements, 239–42; and
 parity, 204–7; and time reversal, 199–201; 204–7
 selection rules for Raman scattering, 237, 388, 410,
 416–17
 spin, 70, 199–200; effective spin, 414
 and torsion vibrations, 368–70
 anomalous polarization, 159–60, 385, 416
 antiHermitian operator, 112–13, 202–3, 219, 387
 antilinear operator, 194
 antioctant rule, 296
 antiStokes Raman scattering, 108–9, 348–9
 antisymmetric scattering, 158–61, 385–407
 in atomic sodium, 385, 394–7
 and degeneracy, 111, 221–2
 in iridium (IV) hexahalides, 397–400
 in porphyrins, 358, 402–7
 and selection rule on Δj , 237, 388; on Δm , 410, 416
 and space-time symmetry selection rules, 386–8
 and spin-flip transitions, 411–14
 and spin-orbit coupling, 410–11
 in uranocene, 416–17
 and vibronic coupling, 401–2
 antiunitary operator, 194
 α -pinene, natural Raman optical activity, 20
 asymmetry, 25
 atom dipole interaction model, 345
 autorotation of the polarization ellipse, 36
 averages of tensor components, 181–5
 axial (pseudo) tensor, 177–80
 axial (pseudo) vector, 29, 177–80
 azimuth, 61–2
 change in refringent scattering, 132–4

 bicyclo-3,3,1-nonan-9-one, magnetic circular
 dichroism, 326
 biomolecules, 10, 381–4
 binaphthyls, infrared circular dichroism, 379–80
 Biot's law of inverse squares, 2
 biphenyls, natural Rayleigh optical activity, 353
 birefringence, 4, 23–4, 127–51
 circular, 4, 141–7, 264–9; *see also* electric,
 magnetic and natural optical rotation
 and circular dichroism
 and coherent forward scattering, 126
 electric field gradient-induced, 138–41
 Jones, 150–1
 linear, 135–7; *see also* Kerr effect
 Bohr magneton, 70, 315, 323
 Boltzmann average, 136, 148
 bond dipole model, 333, 336–40, 362–73
 bond polarizability model, 345, 356–73
 Born–Boys model, 282–4, 350
 Born–Oppenheimer approximation, 114–16, 333, 337
 see also adiabatic approximation
 β -pinene, natural Raman optical activity, 378–9
 broken symmetry, 213–16
 bromochlorofluoromethane CHFCIBr
 absolute configuration, 47, 346
 natural Raman optical activity, 346
 optical rotation, 276, 283

- bulk polarization, quadrupole polarization and magnetization, 266
- carbonyl group
 deformations, natural Raman optical activity, 375–7
 electronic optical activity, 9, 274
 electronic rotational strength, 291–7; vibrational structure in, 307–10
 orbitals and electronic transitions, 292
- Cauchy principal value, 99
- centre of inversion, 188
- charge, electric, 67
- charge conjugation *C*, 33
 violation of, 45–7
- charge transfer transitions, 321, 415–16
- chiral discrimination, 224
- chirality, 2, 25–6
 of atoms, 45
 of elementary particles, 40–1, 44–5, 50, 216
 factor, 287–91
 functions, 243–6; qualitatively complete, 251–6
 homo- and hetero-, 258–61
 index, 258
 and ligand permutation symmetry, 242–63
 numbers, 256–8
 order, 258, 276
 and relativity, 49–50
 true and false, 38–43
 in two dimensions, 50–2
- chiral point groups, 26, 271, 274, 345
- cholesteric liquid crystals, 15, 18
- chromophores, 291
- circular birefringence, 4, 141–7, 264–9
see also electric, magnetic and natural optical rotation and circular dichroism
- circular dichroism, 5–6, 97, 141–7, 264–9
 X-ray, 21–2, 300
see also electric, magnetic and natural optical rotation and circular dichroism
- circular intensity difference, Rayleigh and Raman, 15–16
 electric, 168–9
 magnetic, 21, 166, 408; in porphyrins, 417–20
 natural, 162–3, 342–5, 347–8, 361–2; in model chiral structures, 363–72
- circular polarization of luminescence, 9, 14
- circularly polarized light, 3–4, 61
- closure theorem, 93, 101, 117, 119, 391
- Co(en)₃³⁺, visible, near ultraviolet and X-ray circular dichroism, 297–300
- coherence
 and light scattering and refraction, 124–6
 and polarized light, 64–7
- coherency matrix, 64
- combination scattering, 124
- commutation relations, 82, 93, 102
- complete polarization measurements, 160, 385
- Condon sum rule, 271
- conservation of parity, 33, 189
 in natural and magnetic optical rotation, 33–6
 in natural, magnetic and electric Rayleigh optical activity, 36–8
see also parity
- conservation of time reversal invariance (reversality), 29, 34–6, 38
 in natural and magnetic optical rotation, 33–6
 in natural, magnetic and electric Rayleigh optical activity, 38
see also time reversal
- Coriolis force, 386
- Cotton effect, 6
- Cotton–Mouton effect, 23–4, 137
- Coulomb gauge, 59, 82
- coupling models
 of electronic optical rotation and circular dichroism, 273; static (one electron), 275–6; dynamic (coupled oscillator), 277–85; and Kirkwood's term, 278–82; application to the carbonyl chromophore, 291–7; to hexahelicene, 301–4
 of Rayleigh and Raman optical activity, 350
 of vibrational optical activity in general, 379–80
- coupled oscillator theory, 273, 277–85
 degenerate, 286–91
see also coupling models
- coupling factor, 288–91
- cowpea mosaic virus, natural Raman optical activity, 383–4
- CP* operation, 45–9
- CP* violation, 43, 48–9, 214, 216–17
- CPT* theorem, 43, 48–9, 214, 216–17
- CPT* violation, 49
- crossing relations, 99
- CuBr₄²⁻, magnetic Raman optical activity, 411–14
- degeneracy
 and antisymmetric scattering, 111, 221–2, 386–8
 Kramers, 196
 and magnetic optical activity, 147, 312–16
 and matrix elements of irreducible tensor operators, 238–42
 and parity, 189–93
 and time reversal symmetry, 196–9
- degenerate two-state systems and optical enantiomers, 208–13
- degree of circularity, 66
 due to circular dichroism, 144–5
 as a measure of Rayleigh and Raman optical activity, 140, 348
- degree of polarization, 66
 change in refringent scattering, 132–4; in circular dichroism, 143–5
- depolarization ratio, 156–60
 resonance Rayleigh in atomic sodium, 396–7
 resonance Raman in iridium (IV) hexahalides, 400
- dextro rotatory, 5
- diamagnetic susceptibility, 80, 87
- dielectric constant, 54, 266

- dimethyldibenz-1,3-cycloheptadiene-6-one, methyl torsion Raman optical activity, 373
- dipole moment, *see* electric and magnetic multipole moments
- dipole strength, 270
 vibrational, in fixed partial charge model, 336; in bond dipole model, 339
- direction cosines, 117, 173–8, 182–5, 225–6
- direct product, symmetric and antisymmetric, 199, 235, 387–8
- dispersion forces
 and dynamic coupling, 285
 between odd electron chiral molecules, 224
- dispersion lineshape functions, 96, 105–6
- dissymmetry, 25
- dissymmetry factor, 8, 144, 270
 infrared vibrational, 333; calculations in model chiral structures, 363–72; comparison with Raman circular intensity difference, 362–3
- double groups, 199, 219, 236, 242, 387, 398
- Drude equation, 2
- dyad, 171, 236
- dynamic coupling, 273, 277–85
 Kirkwood's term, 278–85
see also coupling models.
- Einstein summation convention, 172
- electric field gradient-induced birefringence, 138–41
- electric field gradient tensor, 79, 138–9
- electric field vector, 54
 multipole: static, 71–2; dynamic, 76–8; radiated by induced oscillating molecular multipole moments, 126–7
 symmetry of, 32
- electric multipole moments, 67–70
 charge, 67
 dipole, 68, 86, 88; and parity and time reversal, 199, 204–7
 quadrupole, 68–9
- electric optical rotation and circular dichroism, 151
 and conservation of parity and time reversal invariance (reversality), 16, 35
- electric polarizability, 86, 88
 hyperpolarizability, 86
 quadrupole polarizability, 87
- electric Rayleigh and Raman optical activity, 16, 168–9
 and conservation of parity and time reversal invariance (reversality), 37–8
- electromagnetic energy density, 57
- electronic Raman scattering
 in Eu^{3+} , 386
 in uranocene, 414–17
- elliptically polarized light, 5, 36, 61–3
- ellipticity, 5, 46, 61–3
 change in refringent scattering, 132–4; due to birefringence, 135–8; due to circular dichroism, 143, 145, 265–8, 312
 in Rayleigh and Raman optical activity, 14–16, 36–8
- enantiomeric microscopic reversibility, 43
- enantiomers, strict, 46–7
- enantiomorphism, 25
 motion-dependent, 38–43; *see also* false chirality
 time invariant and time noninvariant, 39
- enantioselection, absolute, 23
- ensemble operator, 252
- equation of continuity, 75
- Eu^{3+} , electronic Raman scattering, 386
- Euler angles, 115, 207
- Euler–Lagrange equation, 78
- excitation profile, 155, 403
- exciton
 model of natural electronic optical activity, 286–91
 splitting, 107
- extinction coefficient, 7
- false chirality, 38–43
 and *CP* violation, 49
 and enantiomeric microscopic reversibility, 43
 in two dimensions, 52
- Faraday effect, *see* magnetic optical rotation and circular dichroism
- Faraday *A*-, *B*- and *C*-terms, 312–16
 tensors, 417
- $\text{Fe}(\text{CN})_6^{2-}$, magnetic circular dichroism, 320–4
- FeF_2 , magnetic Raman optical activity, 386
- ferrocytochrome *c*,
 complete Raman polarization measurements, 160–1
 magnetic circular dichroism, 419–20
 magnetic Raman optical activity, 16, 419–22
- fixed partial charge model, 332–6
- fluorescence detected circular dichroism, 9
- fluorine, antiocant behaviour, 296
- Franck–Condon overlap integrals, 306, 391–2
- Fresnel's theory of optical rotation, 3–4
- gauge, Coulomb and Lorentz, 59, 82
- gauge transformation, 58–9
- generalized momentum, 79
- g*-value, 70
 from magnetic Rayleigh and Raman optical activity, 410, 414
 negative, 414
- gyration vector and tensor, 269
- gyrotropic (nonreciprocal) birefringence, 149–50, 224
- haem proteins, 385
- Hamiltonian
 for charged particles in electromagnetic fields, 78–85
 invariance under space inversion, 189; under time reversal, 193
 and symmetry violation, 212–15
- helix, 30–1, 300–4
- Hermitian operator, 112, 202–3, 219
- Herzberg–Teller approximation, 120–2, 305–7, 340, 380–93
see also crude adiabatic approximation
- hexahelicene, dynamic coupling theory of optical rotation, 300–4

- hyperpolarizability, electric, 86
 hydrogen peroxide, chirality of, 192–3
- induced electric and magnetic multipole moments
 dynamic: real, 90–1; complex, 93–4; radiation by, 126–7
 static, 86–7
 improper rotations, 178
 inertial terms in vibrational optical activity, 339, 359, 367–73
 infrared optical rotation and circular dichroism, 17–21, 332–42
 see also vibrational optical activity
 inherently chiral chromophore model, 273–4, 301
 intensity, 57–8
 change in refringent scattering, 132–5
 inverse polarization, 159, 385
 inversion motion in ammonia, 190–2
 inversion symmetry in quantum mechanics, 187–213
 interaction Hamiltonian
 for charged particles with electromagnetic fields, 79–85
 for two charge and current distributions, 81
 intermolecular forces, 224
 IrBr_6^{2-} and IrCl_6^{2-}
 resonance Raman scattering, 397–400
 magnetic Raman optical activity, 411–14
 negative g -value, 414
 irreducible cartesian tensors, 69, 230–8
 irreducible spherical tensor operators, 238–42
 isotropic tensors, 181
- Jahn–Teller effect, 122, 389, 392–3, 404
 Jones birefringence, 150–1
 Jones matrix (calculus) technique, 128–9
 Jones vector, 66–7, 129
 $3j$ symbol, 239
 $6j$ symbol, 395
- Kerr effect, 23–4, 135–7
 Kerr magneto-optic effect, 16
 Kirkwood model of optical rotation, 278–85, 350
 Kramers conjugate, 196
 Kramers degeneracy, 196
 Kramers–Kronig relations, 98–102
 between optical rotation and circular dichroism, 272
 Kramers theorem, 196
 Kronecker delta, 176, 180–1
 Kuhn's dissymmetry factor, *see* dissymmetry factor
 Kuhn–Thomas sum rule, 92–3
- laevo rotatory, 5
 Lagrangian, 78–9
 Laplace's equation, 69
 Levi-Civita (alternating) tensor, 179–81
 lifetimes of excited states, 95
 ligand partitions, 256–8
 light scattering, 14–17, 94, 123–69
 linear birefringence, 135–7
 linear dichroism, 24, 135–7
- linearly polarized light, 3, 61
 linear operator, 194
 lineshape functions, 96, 105–6
 lineshapes for isotropic, anisotropic and antisymmetric scattering, 161
 liquid crystals, 15, 18
 Lorentz condition, 59
 Lorentz factor, 126, 270
 Lorentz force, 57, 78
 Lorentz gauge, 59, 82
 mistaken paternity of, 59
 luminescence, 9, 329
- magnetic field vector, 54
 multipole: static, 72–3; dynamic, 76–8
 symmetry of, 32
 magnetic multipole moments, 70–1
 monopole, 70
 dipole, 70
 quadrupole, 70–1
 magnetic optical rotation and circular dichroism, 10–14, 94, 145–7
 and conservation of parity and time reversal invariance (reversality), 34–5
 symmetry classification of, 201–2
 vibrational, 19–20
 magnetic permeability, 54, 266
 magnetic Rayleigh and Raman optical activity, 16, 20–1, 164–8, 386, 407–22
 and conservation of parity and time reversal invariance (reversality), 37–8
 and g -values, 410, 414
 magnetic susceptibility, 87
 magnetochiral birefringence and dichroism, 21–3, 147–9, 327–9
 symmetry classification of, 202
 and X-ray optical activity, 21
 magnetic symmetry groups, 218
 Maxwell's equations, 54–5
 and conservation laws in electromagnetism, 32
 3-methylcyclohexanone, natural Raman optical activity, 373, 375–7
 methyl group
 vibrational optical activity: in intrinsic modes, 378; in torsions, 367–73
 Mueller matrix (calculus) technique, 128–9
 molecular property tensors, 85–107
 at absorbing frequencies, 95–8
 dynamic: real, 89–92; complex, 93–4; static approximation, 102–3
 origin dependence of, 94
 permutation symmetry of, 219–24
 perturbed, 103–7
 polar and axial, 217–18
 spatial symmetry of, 224–34
 static, 85–8
 symmetry classification of, 217–42
 time-even and time-odd, 217–18
 molecular transition tensors, 107–22
 operators for, 112–14
 permutation symmetry of, 219–24

- moment of inertia, 369–70
- monochromatic waves, 55–6
- multipole interaction Hamiltonians, 79–85
- natural optical rotation and circular dichroism, 2–10, 94, 141–5, 264–310
 - and conservation of parity and time reversal invariance (reversality), 33–6
 - experimental quantities, 269–71
 - of oriented systems, 27–8, 142, 265–9, 281, 297–304
 - vibrational, 17–19, 331–42, 362–80
- natural Rayleigh and Raman optical activity, 14–19, 161–4, 331, 342–84
 - of biomolecules, 381–4
 - bond polarizability model, 356–62
 - and chirality functions, 262–3
 - and conservation of parity and time reversal invariance (reversality), 36–7
 - coupling models, 380
 - experimental quantities, 346–9
 - incident, scattered and dual circular polarization, 348
 - linear polarization, 349
 - magic angle, 348
 - in simple chiral structures, 362–79
 - resonance, 163–4, 348–9
 - spatial symmetry requirements (selection rules) for, 345
 - Stokes–antiStokes asymmetry in, 348–9
 - two-group model, 351–6, 363–7
 - and vibrational optical activity, 17–20
- negative g -value, 414
- Neumann's principle, 217–19
- neutral K -meson, 45, 48, 216–17
- neutrinos, 43–4, 48, 50
- nonreciprocal (gyrotropic) birefringence, 149–50, 224
- normal vibrational coordinates, 115, 121, 334
 - matrix elements of, 334
 - transformation to cartesian atomic displacements, 334; to local internal coordinates, 336
- octant rule, 9, 291–7
- one electron (static coupling) model, 273, 275–6
- optical activity
 - of chiral surfaces, 51
 - definition, 1
 - in light scattering, 14–17
 - magnetic electronic, 311–27
 - magnetic Rayleigh and Raman, 385, 407–22
 - natural electronic, 264–310
 - natural vibrational, 331–84
 - parity and reversality classification of observables, 201–7
 - in reflection, 51
 - review of phenomena, 1–52
 - symmetry and, 24–38
- optical activity tensors, 94
 - for axial symmetry, 187
 - effective operators for, 113, 203
- invariants, 347
 - permutation symmetry of, 223–4
 - symmetry classification of, 217–42
 - transition, 110, 120, 345, 360
- optical rotation, 2–5, 141–7, 264–8
 - see also* electric, magnetic and natural optical rotation and circular dichroism
- optical rotation angle, 2–5
 - Buckingham–Dunn equation for, 142
 - Rosenfeld equation for, 143
- optical rotatory dispersion, 2, 5, 6–7, 11–13
- orbital angular momentum, 29–31, 70, 200–1
- origin dependence (and invariance)
 - of bond dipole vibrational rotational strength, 338–40
 - of bond polarizability Raman optical activity, 357–61
 - of electric dipole moment, 68
 - of electric field gradient-induced birefringence, 138, 141
 - of electric quadrupole moment, 68, 94
 - of exciton optical activity, 287
 - of generalized rotational strength, 270
 - of Kirkwood's term, 279
 - of magnetic dipole moment, 70, 94
 - of molecular property tensors, 94
 - of natural optical rotation and circular dichroism observables, 142, 265, 280–1
- oscillator strength, 92
- paramagnetic susceptibility, 87
- parity P , 28–33
 - and angular momentum quantum states, 204–7
 - classification of operators and observables, 189–90
 - conservation law, 189
 - intrinsic, 188
 - mixed, 189–90
 - operator, 187–8
 - and optical activity observables, 33–8, 192, 201–7
 - and permanent electric dipole moments, 190, 204–7
 - and resolved chiral molecules, 190–3, 207–13
 - of spherical harmonics, 190
- parity violation
 - and optical rotation in free atoms, 45–6, 206
 - and optical enantiomers, 207–13
 - distinction from parity breaking, 214
- partial polarization, 64–7
- partition diagram, 256–7
- permeability, 54
- permittivity, 54
- permutation symmetry
 - and chirality, 242–63
 - of molecular property tensors, 219–24
- permutation group, 246–51
- perturbation theory
 - degenerate, 104, 122, 208–13
 - time-dependent, 89
 - time-independent, 87–8

- 1-phenylethylamine and 1-phenylethanol, natural
Raman optical activity, 16
- photon's magnetic field, nonexistence of, 49
- Placzek's approximation, 116–20, 356, 388
- plane waves, 55–6, 61, 77
- Poincaré sphere, 67
- Poisson's equation, 59
- polarizability tensor
at absorbing frequencies, 94–8
anisotropy, 186–7
dynamic: real, 91; complex, 93; static
approximation, 102–3
effective operators for, 112
invariants, 156, 160, 186, 347
Kramers-Kronig relations between dispersive and
absorptive parts, 98–102
mean (isotropic) part, 186
permutation symmetry of, 219–24
perturbed, 103–7
static, 88
symmetric and antisymmetric parts, 92, 219–24
transition, *see* transition polarizability tensor
- polarization density matrix, 64
- polarization tensor, 64
- polarization vector, 61–2
- polarized light, 61–7
- polar (true) tensor, 177–80
- polar (true) vector, 29, 177–80
- Poynting vector, 57
- porphyrins
antisymmetric scattering, 385, 402–7
magnetic circular dichroism, 317–20
magnetic Raman optical activity, 417–22
resonance Raman scattering, 402–7
- principal axes, 185–7
- principle of reciprocity, 38
- propagation vector, 56
- proper rotations, 178
- proteins
polypeptide backbone, 381–2
natural Raman optical activity, 381–4
- pseudoscalar
quantity, 30–2, 39, 178, 201, 212
particle, 188
- quadrant rule, 294–5, 308
- quadrupole moment, *see* electric and magnetic
multipole moments
- quartz, 2, 18, 26
- quasi-stationary state, 95, 192
- racemic mixture, 27
- Raman electron paramagnetic resonance, 21, 386,
410–17
- Raman optical activity, 14–21, 161–9, 342–84,
407–22
see also electric, magnetic and natural Rayleigh and
Raman optical activity; circular intensity
difference; vibrational optical activity
- Raman scattering, 14
coherence properties of, 124–6
electronic, 386, 414–17
lineshapes, 161
polarization phenomena in, 151–69
resonance, 21, 385–422
rotational, 117–18
Stokes and antiStokes, 108–9, 348–9
vibrational, 116–20
see also antisymmetric scattering
- Raman transition tensors, 116–20, 388–93
- Rayleigh optical activity, 14–17
see also electric, magnetic and natural Rayleigh and
Raman optical activity; circular intensity
difference
- Rayleigh scattering, 14
coherence properties of, 123–6
polarization phenomena in, 151–69
resonance, 393–7
see also antisymmetric scattering
- reduced matrix element, 239, 323, 394–6
- reflection, optical activity in, 51
- refraction, 94, 124, 265–9
- refractive index, 4, 55–6, 131, 148, 265–6
- refrigent scattering, 129–51
- relativity and chirality, 49–50
- response functions, 98
- retarded potentials, 61
- reversal coefficient, 158–9, 385
- reversality
see conservation of time reversal invariance
- Rosenfeld equation, 265
- rotation of axes, 173–7
- rotation group, 235
- rotations, proper and improper, 178
- rotational strength, 270
of carbonyl group, 293–7, 308–10
dynamic coupling, 285
exciton, 287
of oriented samples, 270
origin dependence of, 270
static coupling (one electron), 276
sum rules for, 271–2
vibrational: 332; in fixed partial charge model, 336;
in bond dipole model, 339
vibronically perturbed; 305–7; of carbonyl group,
307–10
- rotatory ether drag, 36
- scalar quantity, 29, 171–3, 178
pseudo-, 30–2, 39, 178, 201, 212
- scalar particle, 188
- scalar potential, 58–60
- scalar product, 171, 178
- scattering tensor, 127
- Schrödinger equation
time-dependent, 89–90; and time reversal,
193–4
time-independent, 87–8, 114–15
- second harmonic scattering, 51
- sector rules, 9, 258, 294–6, 308

- selection rules
 angular momentum, for Raman scattering, 237, 388, 409–10
 for electric dipole transitions in atoms, 240
 generalized space-time, for matrix elements, 198–9;
 application to molecule-fixed electric and magnetic dipole moments, 199; to symmetric and antisymmetric Rayleigh and Raman scattering, 387–8
 spatial, for natural optical rotation, 27, 228–9, 270–1, 274; for natural Rayleigh and Raman optical activity, 163; for magnetochiral birefringence and dichroism, 329
- Sellmeier's equation, 5
- sodium, atomic
 magnetic Rayleigh optical activity, 408–11
 resonance Rayleigh scattering, 394–7
- specific ellipticity, 7
- specific rotation, 7, 269–70
 ab initio computations of, 272
 of hexahelicene, 302–4
- spherical harmonics
 parity of, 190
 phase convention for, 200, 240–1
- spherical tensor operators, 238–43
- spin angular momentum, 70, 200
 effective, 414
- spin-orbit coupling, 224, 322, 394, 410
 and antisymmetric scattering, 409–10
 in atomic sodium, 394–7
 in iridium (IV) hexahalides, 398–400
- spontaneous symmetry breaking, 215
- Stark effect
 in atomic hydrogen, 190
 in symmetric top molecules, 207
- static coupling (one electron) model, 273, 275–6
- stationary states, 89, 95, 193
 and optical enantiomers, 208–13
 and parity violation, 213
 quasi-, 95, 192
- Stokes parameters, 62–7
- Stokes Raman scattering, 108–9, 348–9
- sum rules
 Condon, 271
 and Kramers–Kronig relations, 100–2
 Kuhn–Thomas, 92, 100
 for the rotational strength, 271–2
- symmetric scattering, 155–8
- symmetry matrices, 226
- symmetry and optical activity, 24–52
- symmetry violation, 43–50, 208–17
see also charge conjugation; parity; and time reversal
- tartaric acid, 2, 26–8, 192
- tensor, 29, 171–3
 alternating (Levi-Civita), 179–81
 averages, 181–5
 cartesian, 170–87
 invariants (isotropic tensors), 156, 181, 183–5, 347
 irreducible: cartesian, 69, 230–8; spherical (operators), 238–42
 Kronecker delta, 176, 180–1
 polar (true) and axial (pseudo), 177–80, 217, 226
 rank of, 172
 symmetric and antisymmetric, 173, 236–7
 time-even and time-odd, 217
 unit, 180–1
- time reversal T , 29–33, 193–201
 and angular momentum quantum states, 199–201, 204–7
 classification of molecular property tensors, 217
 classification of operators, 197
 and matrix element selection rules, 197–9
 operator, 193
 and permanent electric dipole moments, 204–7
 violation, 47–9
- torsion vibrations, 365–7, 367–73
- trans-2,3-dimethylloxirane, natural Raman optical activity, 373
- transition optical activity tensors, 110, 120, 345, 360
- transition polarizability tensor, 108–14
 effective operators for, 112–13
 ionic and electronic parts, 119–20
 permutation symmetry of, 219–22
 in Placzek's approximation, 116–20
 symmetric and antisymmetric parts, 110–12, 120, 219–22
 vibronic development of, 388–93; antisymmetric, 401–2
- tunnelling splitting, 192, 212
- two-group model
 of optical rotation and circular dichroism, 274–91
 of Rayleigh optical activity, 351–6
- uncertainty principle and resolved enantiomers, 192–3
- unitary operator, 194
- units, 1
- unit tensors, 180–1
- uranocene, electronic resonance Raman scattering and magnetic Raman optical activity, 414–17
- universal polarimetry, 28
- V coefficients, 240–2
- vector, 29, 171–2
 polar (true) and axial (pseudo), 29, 177–80, 217
 time-even and time-odd, 30, 217
- vector potential, 58–60
- vector product, 178–9
- velocity–dipole transformation, 93–4
 vibrational, 335
- Verdet constant, 10
- Verdet's law, 10
- vibrational optical activity
 magnetic, 19–21, 407–22
 natural, 17–19, 331–84
- vibrational rotational strength, 332

Index

443

- in fixed partial charge model, 336
- in bond dipole model, 339
- vibrational structure in circular dichroism spectra, 304–10
- vibronic coupling, 120–2, 305–7, 388–93
 - and antisymmetric scattering, 401–2
- viruses, natural Raman optical activity, 383–4
- wavevector, 56
- wave zone, 77
- weak neutral current, 45, 211–12
- Wigner–Eckart theorem, 239–42
- X-ray optical activity, 21–2
 - in Co(en)_3^{3+} , 300
 - and magnetochiral dichroism, 21
- Young diagram, 248
- Young operator, 251
- Young tableau, 249–51
- Zeeman effect, 11–12, 107, 313
 - and the Faraday *A*-, *B*- and *C*-terms, 314–16
 - and magnetic Rayleigh and Raman optical activity, 409–16
 - and the magnetochiral *A*-, *B*- and *C*-terms, 329