

# INDEX

- A**, vector potential, 4  
**A** terms, MCD, first derivative of bandshape, 20ff  
**A** terms, MLD, second derivative of bandshape, 189  
**A** term parameter  $A_1$ , 20ff  
  oriented case, 18, 19  
  space averaged case, 20  
**A** term parameter ratio  $A_1/D_0$ , 22  
Absorbance,  $A$ , 1  
Absorptivity, molar  $\epsilon$ , 1, 13  
Absorption coefficient, 10–11, 12–13  
Absorption probabilities, 10ff  
Acetylene,  $C_2H_2$ , gas phase. *See* MVCD spectra  
Alternating tensor, definition, 19, 50  
Atomic Hg vapor. *See* MCD spectra and MLD spectra  
Au. Colloidal gold. *See* MCD spectra  
 $AuCl_2^-$ . *See* MCD spectra  
 $Au(AuPPh_3)_8^{3+}$ . *See* MCD spectra  
 $AuX_4^-$ ,  $X = Cl^-, Br^-$ . *See* MCD spectra  
Axial distortions, 136, 142, 159  
Azurin, *Pseudomonas aeruginosa* blue copper protein. *See* MCD spectra  
Azurin, *Pseudomonas aeruginosa* Nickel(II) Azurin (NiAz). *See* XMCD spectra
- B** band for phthalocyanine complexes, 112, 113, 116  
**B**, magnetic flux, 4, 5  
**B** terms, 26ff  
**B** term parameter  $B_0$ , 27  
  oriented case, 18  
  space averaged case, 20  
Basis functions, standard basis, 48  
Bandshape function, 10  
Beer–Lambert law, 1  
Benzene  $C_6H_6$  vapor. *See* MCD spectra  
Benzene, matrix isolated. *See* MCD spectra
- Benzene vapor, vacuum UV. *See* MCD spectra  
Birefringence, 6, 42  
Born–Oppenheimer approximation, 14  
BO–FC–RS approximation, 16, 18
- C** terms, 24ff  
**C** term parameter  $C_0$ , 24  
  oriented case, 18, 19  
  space averaged case, 20  
  temperature dependence, 24  
**C** term parameter ratio  $C_0/D_0$ , 25  
 $C_4(Me_3Si)_4^{2-}$ . *See* MCD spectra  
 $C_2H_2$ , gas phase. *See* MVCD spectra  
 $CH_4$ , gas phase. *See* MVCD spectra  
CO, gas phase. *See* MVDC spectra  
Calibration, 42  
Case studies, MCD **A** and **B** terms for diamagnetic systems, 60  
  atomic mercury vapor, 61  
  benzene:  $\pi \rightarrow \pi^*$  and Rydberg transitions, 103  
   $D_{4h}$  cyclobutadiene dianion  $Li_2[C_4(Me_3Si)_4]$ , 109  
  chlorophyll *Q* band, an example using **B** terms, 116  
  linear two coordinate  $D_{\infty h}$  complexes:  $d \rightarrow s$ , LMCT and MLCT transitions, 75  
  metal cluster complexes: MLCT, metal centered, and IF transitions, 86  
  methyl iodide:  $n \rightarrow \sigma^*$  and iodine based Rydberg transitions, 99  
  octahedral complexes, 80  
  sodide  $Na^-$  ion, 63  
  square complexes of  $D_{4h}$  symmetry: LF, LMCT, MLCT and  $d \rightarrow p$  transitions, 64  
  surface plasmon band for colloidal gold nanoparticles, 119

- triiodide ion, pseudo A term  
example, 97
- zinc phthalocyanine complex  $\text{ZnPc}(2-)$ ,  
111
- Case studies, MCD C terms for  
paramagnetic systems, 121
- blue copper protein *Pseudomonas*  
*Aeruginosa* Azurin, ODEPR, 150
- $\text{Co}^{2+}$  as a probe of binding sites in  
*E. Coli* Methionyl Aminopeptidase,  
146
- cyano complexes, LMCT, 121
- cyclooctatetraene mononegative ion  
 $\text{COT}^-$ , matrix isolated, 131
- Mn(II) phthalocyanine, ground state  
determination, 129
- lanthanide ions in crystalline environ-  
ments, 162
- multicopper oxidase, modeling NI from  
*Rhus vernicifera* Laccase, 138
- non-heme iron enzymes, variable  
temperature and field  
studies, 135
- protein oxidized Rubredoxin, *Desulfovi-*  
*brio Gigas*, 142
- single molecule magnets SMM, 155
- unstable metallocenes, ground state  
magnetization, 127
- Case studies (examples), MVCD, 173
- acetylene and deuterated isotopomers,  
rotationally resolved spectra, 176
- carbon monoxide, rotationally resolved  
spectra, 174
- $\text{M}(\text{CO})_6$ ,  $\text{M} = \text{Cr}, \text{Mo}, \text{and } \text{W}$ , 173
- methane, rotationally resolved spectra,  
176
- Case studies, XMCD, 180–187
- $\text{GdNi}_2$  Laves phase, 180
- Mn(III) and Mn(IV) in SMM, 184
- Pseudomonas Aeruginosa* Nickel(II)  
Azurin (NiAz), 187
- $\text{Sr}_2\text{CrReO}_6$  double perovskite, 181
- Case studies, MLD, 192
- atomic mercury vapor, 193
- deoxymyoglobin, 199
- ferrocycochrome *c*, 199
- $\text{Ho}^{3+}$  in aqueous solution, 197
- metal atoms, matrix isolated in  
noble gas matrices, 195
- $\text{CD}_3\text{I}$ . See MCD spectra
- $\text{CH}_3\text{I}$ . See MCD spectra
- Concentration dependence, 1, 13
- $\text{COT}^-$  in an Ar matrix. See MCD spectra
- $\text{Co}^{2+}$  in *E. Coli* Methionyl Aminopeptidase,  
*EcMetAP*. See MCD spectra
- Chain of groups method, 53
- Chlorophyll, Chl-*a*-WSCP. See MCD  
spectra
- Chlorophyll porphyrin complex, 117
- Circular polarization, 5ff
- Circular dichroism (CD), 1, 8–9
- Coefficients of fractional parentage,  
definition, 52–53
- $(\text{CN})\text{ZnPc}(2-)$ . See MCD spectra
- Colloidal gold. See MCD spectra
- Coordinate systems, 18
- Coordinate origin change for angular  
momentum operators, 19
- Copper protein, azurin, *pseudomonas*  
*aeruginosa* blue copper protein.  
See MCD spectra
- Coulomb gauge, 4
- Coupling coefficients,  $3j_m$ , 47
- Coupling coefficients,  $6j$ , 48
- $[\text{Cr}_{12}\text{O}_9(\text{O}_2\text{CCMe}_3)_{15}]$ . See MCD spectra
- $\text{Cu}(\text{II})$  trisOH. See MCD spectra
- $\text{Cu}(\text{II}) \mu_3\text{O}$ . See MCD spectra
- $d \rightarrow p$  transitions, 66, 73, 75, 82, 84
- $d \rightarrow s$  transitions, 75, 77
- Data acquisition, 40
- Delta  $A$ ,  $\Delta A$ , 1, 18, 40, 188
- Delta  $\epsilon$  for MCD per unit field,  $\Delta\epsilon_M$ , 1, 40
- Deoxymyoglobin. See MLD spectra
- Depolarization, 42
- Detector signals, measurement of  $A$  and  
 $\Delta A$ , 38
- Deviation from the linear limit, 31
- Diamagnetic systems:  $A$  and  $B$  terms, 60
- Dichroism, 1, 188
- Dipole strength parameter  $D_0$ , 18
- oriented case, 18
- space averaged case, 20
- Dipole moment operator, 11
- E. Coli* Methionyl Aminopeptidase,  
*EcMetAP*. See MCD spectra
- Electric dipole transitions, 12
- Electric quadrupole, 11, 12
- Electronic degeneracy, 16
- Elliptically polarized light, 8–9
- Ellipticity, molar,  $[\theta]$ , 3, 40
- Energy level diagrams
- benzene  $\pi$  in  $D_{6h}$  symmetry, 104
- calculated spin-orbit states for  
 $\text{Pt}(\text{CN})_4^{2-}$ , 72

- Energy level diagrams (*Continued*)  
 COT<sup>-</sup>  $\pi$  electrons, 132  
 Cr<sup>III</sup>O<sub>6</sub> electronic states, 162  
 cyclobutadiene dianion, 109  
 $D_{2d}$  symmetry M(CN)<sub>8</sub><sup>n-</sup>, 126  
 $D_{3h}$  symmetry Hg<sub>3</sub><sup>4+</sup> metal centered orbitals, 91  
 $D_{3h}$  symmetry Pt<sub>3</sub>(CO)<sub>3</sub>(P(*t*-Bu)<sub>3</sub>)<sub>3</sub>, 88  
 $D_{4d}$  symmetry Pt(AuPPh<sub>3</sub>)<sub>8</sub><sup>2+</sup> ion, 94  
 $D_5$  symmetry  $d^4$  Cp<sub>2</sub>Mo and Cp<sub>2</sub>W, and  $d^5$  Cp<sub>2</sub>Re, 128  
 $^4E_g(e_g^3 a_{1g} b_{2g})$  ground state, 131  
 for an  $nd^8 D_4$  metal complex, 54, 67  
 for linear ( $D_{\infty h}$ ) MX<sub>2</sub> halide complexes, 75  
 for octahedral halo complexes, 81  
 ground state splitting for 6 coordinate and 5 coordinate Co<sup>2+</sup>, 149  
 ground state spin sublevels for  $S = 10$ , 157  
 high spin  $3d^5$  Fe(III) in  $D_{2d}$  symmetry, 143  
 LMCT for Fe(CN)<sub>6</sub><sup>3-</sup>, 123  
 LF transitions for a square  $D_{4h}$  complex, 64  
 LMCT transitions for a square  $D_{4h}$  complex, 67  
 linear Pt(PBu<sub>3</sub>)<sub>2</sub>, 79  
 MLCT transitions for Pt(CN)<sub>4</sub><sup>2-</sup>, 71  
 $nd^6$  M(CO)<sub>6</sub> and M(CN)<sub>6</sub><sup>4-</sup> complexes, 84  
 $^1P_{0,\pm 1} \rightarrow ^1S_0$ , 24  
 $5p$  MO's for I<sub>3</sub><sup>-</sup>, 97  
 $s \rightarrow p_x$  and  $p_y$  crystal field, 27  
 $s^2 \rightarrow sp$ ,  $^1S_0 \rightarrow ^1P_{0,\pm 1}$ , 21  
 Schematic for CH<sub>3</sub>I, 100  
 Zeeman levels for  $^1S_0 (s^2) \rightarrow ^1P_{0,\pm 1} (sp)$ , MCD and MLD transitions, 190  
 zero field splitting for an  $S = 2$  ground state, 137  
 ZnPc(2-), 113  
 EPR silent paramagnetic systems, study by MCD C terms, 127, 137  
 Evaluation of matrix elements, 51ff  
 reduced matrix elements, RME's, 51  
 matrix elements for LCAO MO functions, 55  
 Eu(ODA)<sub>3</sub><sup>3-</sup>, ODA = O<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>O<sub>2</sub><sup>2-</sup>.  
*See* MCD spectra  
 Faraday effect, magnetic optical rotation, 1  
 Fe(CN)<sub>6</sub><sup>3-</sup>. *See* MCD spectra  
 Ferrocyclochrome *c*. *See* MLD spectra  
 Franck-Condon approximation, 14  
 Function, spatial average, 19  
 Function transformation coefficients, 48  
 $g$  factor, 21  
 Gaussian lineshape, 33  
 Gaussian units, 4  
 GdNi<sub>2</sub>,  $L_3$  and  $L_2$ . *See* XMCD spectra  
 GdNi<sub>2</sub>,  $M_5$  and  $M_4$ . *See* XMCD spectra  
 Ground state near degeneracy, 30  
 Group theory, 47ff  
 Group-subgroup chains, *see* chain of groups method, 53  
**H**, magnetic field strength, 4  
 Hamiltonian, 145, 163  
 Herzberg-Teller vibronic approximation, 59, 66, 77  
 Hg vapor. *See* MCD spectra; *and see* MLD spectra  
 HgX<sub>2</sub>, X = Cl<sup>-</sup>, Br<sup>-</sup>, and I<sup>-</sup>. *See* MCD spectra  
 Hg<sub>3</sub>(dppm)<sub>3</sub><sup>4+</sup>. *See* MCD spectra  
 Ho<sup>3+</sup> in aqueous solution. *See* MLD spectra  
 Hole configuration, 53  
 Hysteresis of magnetization, 155-156, 159, 182  
 Hysteresis of MCD intensity due to spin polarization, 158  
 Hot bands, 105, 108  
 I<sub>3</sub><sup>-</sup>, triiodide ion. *See* MCD spectra  
 Intraframework IF transitions in gold cluster complexes, 95-96  
 Intensity, 10  
 Iron enzymes, non-heme, VTVH  $C$  term studies, 135  
 Irreducible tensor methods, 3, 47  
 Irreducible representations (Irreps), 48  
 dimension,  $|a|$ , 49  
 irrep partners, 48  
 Isotropic molecules, oriented case, 20  
 $J$ , total spin and orbital angular momentum, 21, 195  
 Jahn-Teller effect, 112-113, 132, 134  
 Kramers pairs, 25  
 KY<sub>3</sub>F<sub>10</sub>(Eu<sup>3+</sup>). *See* MCD spectra  
 $L$ , total orbital angular momentum, 15  
 Laccase, *Rhus vernicifera*, multicopper oxidase, 138

- Landé formula for  $g$  factors, 21  
 LCAO MO functions, matrix elements, 55  
 LiErF<sub>4</sub>. *See* MCD spectra  
 Ligand field LF transitions for PtCl<sub>4</sub><sup>2-</sup>, 65  
 Ligand to metal charge transfer LMCT transitions, 66, 67, 75, 78, 80, 82  
 Linear dichroism, 188  
 Linear limit, 15  
 Linear polarization, 5  
 Lineshape function, 17  
 LiYF<sub>4</sub>(Eu<sup>3+</sup>). *See* MCD spectra  
 Lock-in amplifier, LIA, 37, 39  
 Lorentz effective field approximation, 11
- Magnetic circular dichroism (MCD), 1  
 Magnetic dipole, 12  
 Magnetic field strength, **H**, 4  
 Magnetic field flux, **B**, 4  
 Magnetic linear dichroism (MLD), 188  
 Magnetic moment, 20, 22, 24, 52, 83, 103, 120, 150–151, 171, 173, 176, 180–182, 185, 187  
 Magnetic optical rotation, 1  
 Magnetic optical rotatory dispersion  
 MORD, 2  
 Magnetic vibrational circular dichroism (MVCD), 171  
 instrumentation, 172  
 examples, 173  
 Magnetization hysteresis, 155–156  
 Magnet systems, 43  
 superconducting, 43ff  
 field orientation, 36, 45  
 Matrix element evaluation, 51, 55  
 MCD spectrometer, block diagram, 37  
 MCD parameters, 20  
 oriented (isotropic) case, 18, 20  
 space averaged case, 20  
 MCD spectra, for specific samples  
 atomic Hg vapor, 61  
 AuCl<sub>2</sub><sup>-</sup>, 76  
 Au(AuPPh<sub>3</sub>)<sub>8</sub><sup>3+</sup>, 95  
 AuX<sub>4</sub><sup>-</sup>, X = Cl<sup>-</sup>, Br<sup>-</sup>, 68  
 azurin, *pseudomonas aeruginosa* blue copper protein, 155  
 benzene C<sub>6</sub>H<sub>6</sub> vapor, 104, 106  
 benzene, matrix isolated, 106, 107  
 benzene vapor, vacuum UV, 108  
 BiCl<sub>6</sub><sup>3-</sup>, 83  
 CD<sub>3</sub>I, 102  
 CH<sub>3</sub>I, 101  
 C<sub>4</sub>(Me<sub>3</sub>Si)<sub>4</sub><sup>2-</sup>, 110  
 (CN)ZnPc(2-), 114  
 chlorophyll, Chl-*a*-WSCP, 118  
 colloidal gold, 119  
 COT<sup>-</sup> in an Ar matrix, 133  
 [Cr<sub>12</sub>O<sub>9</sub>(O<sub>2</sub>CCMe<sub>3</sub>)<sub>15</sub>], 161  
 Co<sup>2+</sup> in *E. Coli* Methionyl Aminopeptidase, *EcMetAP*, 147  
 Eu(ODA)<sub>3</sub><sup>3-</sup>, ODA = O<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>O<sub>2</sub><sup>-</sup>, 164  
 Fe(CN)<sub>6</sub><sup>3-</sup>, 122  
 HgX<sub>2</sub>, X = Cl<sup>-</sup>, Br<sup>-</sup>, and I<sup>-</sup>, 77  
 Hg<sub>3</sub>(dppm)<sub>4</sub><sup>4+</sup>, 91  
 I<sub>3</sub><sup>-</sup>, 98  
 KY<sub>3</sub>F<sub>10</sub>(Eu<sup>3+</sup>), 169  
 LiErF<sub>4</sub>, 168  
 LiYF<sub>4</sub>(Eu<sup>3+</sup>), 169  
 M(CN)<sub>6</sub><sup>4-</sup>, M = Fe(II), Ru(II), and Os(II), 86  
 M(CN)<sub>8</sub><sup>3-</sup>, M = Mo(V) and W(V), 125  
 MnPc in Ar matrix, 130  
 [Mn<sub>12</sub>O<sub>12</sub>(O<sub>2</sub>CC<sub>14</sub>H<sub>29</sub>)<sub>16</sub>(H<sub>2</sub>O)<sub>4</sub>], Mn<sub>12</sub>C<sub>15</sub> SMM, 158  
 Na<sup>-</sup> (sodide) ion, 63  
 Nd(ODA)<sub>3</sub><sup>3-</sup>, ODA = O<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>O<sub>2</sub><sup>-</sup>, 166–167  
 protein oxidized rubredoxin from *Desulfovibrio gigas*, 144  
 Pt(AuPPh<sub>3</sub>)<sub>8</sub><sup>2+</sup>, 94, 96  
 PtCl<sub>4</sub><sup>2-</sup>, 65, 69  
 PtCl<sub>6</sub><sup>4-</sup>, 81  
 Pt(CN)<sub>4</sub><sup>2-</sup>, 70  
 Pt(en)<sub>2</sub><sup>2+</sup>, 74  
 Pt(PBu<sub>3</sub>)<sub>2</sub>, 78  
 Pt<sub>3</sub>(CO)<sub>3</sub>(P(*t*-Bu)<sub>3</sub>)<sub>3</sub>, 87  
 ruby, ODEPR, 153  
 SbCl<sub>6</sub><sup>-</sup>, 82  
 SnCl<sub>6</sub><sup>2-</sup>, 82  
 trinuclear copper NI laccase, 139  
 trinuclear Cu(II) trisOH, 140  
 trinuclear Cu(II) μ<sub>3</sub>O, 141  
 W(CO)<sub>6</sub>, 85  
 M(CN)<sub>6</sub><sup>4-</sup>, M = Fe(II), Ru(II), and Os(II).  
*See* MCD spectra  
 M(CN)<sub>8</sub><sup>3-</sup>, M = Mo(V) and W(V). *See* MCD spectra  
 M(CO)<sub>6</sub>, M = Cr, Mo, and W, 84  
 MCD, MLCT transitions, 84  
 MVCD, 174  
 Metal to ligand charge transfer MLCT transitions, 66  
 Metal centered transitions  
 $d \rightarrow p$ , 66, 73, 75, 82, 84  
 $d \rightarrow s$ , 75, 77  
 $d \rightarrow d$ , LF, 65, 80

- Metal centered transitions (*Continued*)  
 intraframework, IF, in cluster complexes, 95  
 Rydberg. *See* Rydberg transitions  
 $s \rightarrow p$ , 82
- Methane, CH<sub>4</sub>, gas phase. *See* MVCD spectra
- Methyl iodide, CH<sub>3</sub>I and CD<sub>3</sub>I. *See* MCD spectra
- MLD spectra  
 atomic Hg vapor, 193  
 deoxymyoglobin, 201  
 ferrocycochrome *c*, 200  
 Ho<sup>3+</sup>, 198–199  
 Ni atoms, matrix isolated in Ar, 197
- MnPc in Ar matrix. *See* MCD spectra
- Mn<sub>12</sub>Ac cluster. *See* XMCD spectra
- [Mn<sub>12</sub>O<sub>12</sub>(O<sub>2</sub>CC<sub>14</sub>H<sub>29</sub>)<sub>16</sub>(H<sub>2</sub>O)<sub>4</sub>], Mn<sub>12</sub>C<sub>15</sub>SMM. *See* MCD spectra
- Modulator. *See* photoelastic modulator PEM, 36
- Molar ellipticity [ $\theta$ ]<sub>M</sub>, 1, 40
- Moments, method of, 34–35  
 moments of absorption spectra, 35  
 moments of MCD spectra, 35
- MVCD spectra  
 CH<sub>4</sub>, gas phase, 177  
 C<sub>2</sub>H<sub>2</sub>, gas phase, 178  
 CO, gas phase, 175  
 Mo(CO)<sub>6</sub> in CCl<sub>4</sub> solution, 174
- $n \rightarrow \sigma^*$  transitions, 99
- Na<sup>-</sup> (sodide) ion. *See* MCD spectra
- Nanoparticle colloidal gold, 119
- Natural CD. *See* circular dichroism (CD)
- Nd(ODA)<sub>3</sub><sup>3-</sup>, ODA = O<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>O<sub>2</sub><sup>2-</sup>.  
*See* MCD spectra
- Nested magnetization curves, 129, 136, 145, 148–149
- Ni atoms, matrix isolated in Ar. *See* MLD spectra
- Ni(II) azurin, NiAz. *See* XMCD spectra
- Normal modes, 77, 105, 173, 176–177
- Octahedral complexes, 80
- ODEPR, optical detection of electron paramagnetic resonance, 150ff
- One-centered approximation, 55
- Operators, 11
- Operator and function transformation  
 coefficients, 202ff  
 groups *O* and *T<sub>d</sub>* tables, 202  
 groups *D<sub>4</sub>* tables, 207  
 groups *D<sub>3</sub>* tables, 209
- Optical elements for the MCD measurements, 41–42
- Optical rotation, of plane polarized light, 6–7
- Oriental averaging, 19
- $\pi \rightarrow \pi^*$  transitions, 103, 110, 112  
 benzene, 103  
 cyclobutadiene, 110  
 phthalocyanine complexes, 112–113
- Paramagnetic systems: *C* terms, 121
- Parameter evaluation, 34  
 lineshape functions, 34  
 method of moments, 34–35
- Partners, of irreps, 48
- Phase factors, *2jm* and *3jm*, 48
- Photoelastic modulator, PEM, dynamic wave plate, 36
- Phthalocyanine (tetraazotetraphenylporphyrin) complexes, 111, 129
- Piepho and Schatz book, xi, 2–3
- Polarization vector, 5
- Polarized light, 4  
 circular, 5  
 linear, 4–5  
 plane, 4–5  
 rotation of plane polarized light, 7
- Poyting vector, 10
- Protein oxidized rubredoxin from *Desulfovibrio gigas*. *See* MCD spectra
- Pseudo *A* term, 29  
 from *B* terms, 27, 29  
 from *C* terms, temperature dependent, 30
- Pt(AuPPH<sub>3</sub>)<sub>3</sub><sup>2+</sup>. *See* MCD spectra
- PtCl<sub>4</sub><sup>2-</sup>. *See* MCD spectra
- PtCl<sub>6</sub><sup>2-</sup>. *See* MCD spectra
- Pt(CN)<sub>4</sub><sup>2-</sup>. *See* MCD spectra
- Pt(en)<sub>2</sub><sup>2+</sup>. *See* MCD spectra
- Pt(PBu<sub>3</sub>)<sub>2</sub>. *See* MCD spectra
- Pt<sub>3</sub>(CO)<sub>3</sub>(P(*t*-Bu)<sub>3</sub>)<sub>3</sub>. *See* MCD spectra
- Q* band, 100, 112, 116  
 phthalocyanine complexes, 112–116  
 chlorophyll porphyrin complexes, 116  
 $n \rightarrow \sigma^*$  transitions for methyl iodide, 100
- Reduced matrix element (RME), 47  
 matrix element evaluation, 55–56  
 MCD parameters in terms of RME's, 48–50

- Relative magnitude  
 MCD *A*, *B*, and *C* terms, 33  
 MLD terms, 190
- Rigid shift (RS) approximation, 16ff
- Rhombic distortions in ground state,  
 136–137, 142, 159
- Rotation–vibration transitions in MVCD,  
 rotationally resolved MVCD, 174  
 CH<sub>4</sub>, 176  
 C<sub>2</sub>H<sub>2</sub> and deuterated isotopomers, 176  
 CO, 174
- Rubredoxin from *Desulfovibrio gigas*,  
 protein oxidized from. *See* MCD  
 spectra
- Ruby, ODEPR. *See* MCD spectra
- Rydberg transitions, 99, 100–102, 108
- Saturation effects, 31–32
- SbCl<sub>6</sub><sup>-</sup>. *See* MCD spectra
- Selection rules, 22, 175, 188
- Single-molecule magnets,  
 SMM's, 155
- 6*j* coefficients, 48  
 groups *O* and *T<sub>d</sub>* tables, 205  
 group *D<sub>4</sub>* tables, 208  
 group *D<sub>3</sub>* tables, 210
- SnCl<sub>6</sub><sup>-</sup>. *See* MCD spectra
- S, total spin angular momentum, 15
- Spatially averaged case, 20
- Spectrometer for MCD measurements,  
 diagram, 36–37
- Spin magnetic moment, 57
- Spin–orbit coupling, 57
- Spin–orbit secular determinants for *D<sub>4h</sub>*  
 MLCT states in Pt(CN)<sub>4</sub><sup>2-</sup>, 72
- Sr<sub>2</sub>CrReO<sub>6</sub> double perovskite. *See* XMCD  
 spectra
- Standard basis and other conventions, 3
- Strain birefringence, 42, 45
- Stray polarization effects, 41
- Stray fields, 45
- Sum rules, XMCD, 180
- Surface plasmon band for colloidal gold  
 nanoparticles, 119
- Symmetry group tables of 3*jm*, 6*j* and  
 operator and function irreps  
*O* and *T<sub>d</sub>* tables, 204–206  
*D<sub>4</sub>* tables, 208  
*D<sub>3</sub>* tables, 210
- Tetraazotetrazabenzophorphyrin complexes.  
*See* phthalocyanine complexes
- Temperature dependence, MCD *C* terms,  
 24, 30, 31–32, 121
- 3*j* phase {*abc*}  
*O* and *T<sub>d</sub>* single valued irreps, 203  
*D<sub>4</sub>* single valued irreps, 207  
*D<sub>3</sub>* single valued irreps, 209
- 3*jm* coefficients  
 groups *O* and *T<sub>d</sub>* tables, 204–205  
 group *D<sub>4</sub>* tables, 207  
 group *D<sub>3</sub>* tables, 210
- 3*jm* factor  
 partial list for *SO<sub>3</sub>* ⊃ *O* single valued  
 irreps, table, 211  
 partial list for *O* ⊃ *D<sub>4</sub>* single valued  
 irreps, table, 212
- Transition moment cancelation, 27
- Triiodide ion I<sub>3</sub><sup>-</sup>. *See* MCD spectra
- Trinuclear copper NI laccase. *See* MCD  
 spectra
- Trinuclear Cu(II) trisOH. *See* MCD  
 spectra
- Trinuclear Cu(II) μ<sub>3</sub>O. *See* MCD spectra
- Units  
 absorption, 13, 40  
 angular momentum, 11  
 Gaussian, 4  
 MCD, 3, 40  
 magnetic field, 3, 40
- Unit vectors, 5
- Variable temperature, variable  
 field, VTVH, 135, 139
- Vibronic transitions, 66, 77  
 Herzberg–Teller approximation, 59
- Vector potential, **A**, for describing wave  
 properties of light, 4
- W(CO)<sub>6</sub>. *See* MCD spectra
- Wigner-Eckart theorem and RME's, 47
- X-ray MCD (XMCD) and absorption  
 measurements, 179ff
- XMCD spectra  
 GdNi<sub>2</sub>, *L<sub>3</sub>* and *L<sub>2</sub>*, 182  
 GdNi<sub>2</sub>, *M<sub>5</sub>* and *M<sub>4</sub>*, 183  
 Mn<sub>12</sub>Ac cluster, 185  
 Ni(II) azurin, NiAz, 187  
 Sr<sub>2</sub>CrReO<sub>6</sub>, double perovskite, 184
- Zeeman effect, 1, 188  
 perturbation Hamiltonian, 15, 21  
 splitting > bandwidth, 32  
 sublevels, 21, 24, 190
- Zero field splitting, ZFS, 136, 139, 142,  
 149, 159–162