

# Index

Since the number of compounds included in this volume is numerous, entries for most of individual compounds are collected under general entries such as vibrational frequencies and sulfur compounds. Normal modes of vibration, infrared and Raman spectra included are found under respective general titles.

- Ab initio* calculation of force constants, 106  
 Accidental degeneracy, 58  
 Acoustical branch, 131  
 Aluminosilicates, 278  
 Anharmonicity, 11  
 Anharmonicity corrections, 103, 149  
 Anisotropy of polarization, 92  
 Anomalous polarization (*ap*), 94, 104, 229  
 Antimony compounds, 290  
 Anti-Stokes line, 8  
 Antisymmetric vibration, 29  
 Aragonite, 122  
 Arsenic compounds, 290  
 A-term resonance, 99  
 Axis of symmetry. *p*-fold ( $C_p$ ), 22
- Badger's rule, 14  
 Band assignments, 82  
 Bismuth compounds, 290
- B-matrix, 60  
 Bohr's frequency condition, 1  
 Boron compounds, 254  
 Boron hydrides (boranes), 255  
 Bravais lattices, 117  
 Brillouin zone, 131  
 B-term resonance, 99  
 Buckminsterfullerene ( $C_{60}$ ), 259
- Calcite, 122, 126  
 Carbonate radical ( $CO_3$ ), 181  
 Carbon clusters (small), 258  
 Carbon compounds, 258  
 Carbon oxide anions, 276  
 Cartesian coordinate, 107  
 Center of symmetry (*i*), 22  
 Ceramic superconductors, 136  
 Character ( $\chi$ ), 41  
 Character tables, 355

- Chlorine isotope pattern, 199  
 Class 36  
 Combination bands, 5, 11  
 Correlation method, 124  
 Correlation tables, 119, 127, 393  
 Crystallographic point groups, 116  
 Crystals, vibrational analysis, 119  
 Cubic potential, 11  
 $C_5$ , 258  
 $C_{60}$ , 259  
 $C_{60}$  dimer, 263  
 $C_{70}$ , 264  
 $C_{60}Br_{24}$ , 263  
 $C_{60}K_3$ , 263  
 $C_{84}$ , 265
- Decius formula, 64  
 Degenerate vibration, 26  
 Density functional theory (DFT), 106  
 Depolarization ( $dp$ ), 92  
 Depolarization ratio, 81, 92  
 Diamond, 272  
 Diazene ( $N_2H_2$ ), 189  
 Dichroism, infrared, 134  
 Dipole moment, changes, 31  
 Dispersion curves, 131, 134
- Electromagnetic spectrum, 3  
**E**-matrix, 60  
 Endohedral fullerenes, 267  
 Energy level diagram, 4  
 Excitation profile, 105
- Factor group analysis, 123  
 Fermi resonance, 58  
**F**-matrix, 59, 382  
 Force constants, 10  
 Force field, 71  
 Frank-Condon factor, 100  
 Fundamental vibrations, 5
- Gas phase, infrared spectra, 109  
 Generalized coordinate ( $q$ ), 15  
 Generalized valence force (GVF) field, 72  
 Germanium compounds, 276  
**GF** matrix method, 58  
**GF** matrix elements, 382  
 Glide plane, 118
- G**-matrix, 59, 382  
 Gordy's rule, 14  
 Group, 34  
 Group frequencies, 82  
 Group frequency charts, 286, 292, 388  
 Group theory, 34  
 $g$ -vibration, 34
- Halogeno compounds, 296  
 Harmonic oscillator, 10  
 Herman-Mauguin (HM) notation, 119  
 Hermite polynomial, 11  
 Herschbach-Laurie equation, 15  
 Hot bands, 5  
 Hydronium ( $OH_3^+$ ) ion, 174
- Ice, 168  
 Identity ( $I$ ), 22  
 Improper rotation, 43  
 Inert gas matrix, 109  
 Infrared dichroism, 134  
**Infrared spectra**  
 $B_3N_3H_6$  (borazine), 257  
 $[B_6X_6]Cs_2$ , ( $X = Cl, Br$  and  $I$ ), 256  
 $C_5$ , 260  
 $C_{60}$ , 261  
 $C_{70}$ , 266  
 $C_{84}$ , 267  
 $CaCO_3$  (calcite), 134  
 $[ClO_3]K$ , 179  
 $Cr(CO)_6$ , 111  
 $Eu@C_{74}$ , 268  
 $GeCl_4$ , 199  
 $HArF$ , 173  
 $H_2NCN$  (cyanamide), 283  
 $[IO_3]K$ , 179  
 $MF_6$ , ( $M = Mo, Te, Ru$  and  $Rh$ ), 230  
 $NH_3$ , 4  
 $NH_4Cl$ , 195  
 $NiF_2$ , 163  
 $NNO$ , 174  
 $[OsF_6Cl_{6-n}]^{2-}$ , ( $n = 2\sim 4$ ), 236  
 $[PbF_3]M$  ( $M = Na, K, Rb, Cs$ ), 115  
 $P_4N_4Cl_8$ , 291  
 $Sc(CO)_n$ , 114  
 $Sc_3N@C_{80}$ , 270  
 $Si_6H_{12}$ , 278  
 $SiO_2$  ( $\alpha$ -quartz), 280

- $^{235}\text{UF}_6/^{238}\text{UF}_6$ , 232  
 $\text{US}_n$ , 113  
 $\text{XeF}_4$ , 212  
Inert gas matrices, 109  
Intensity  
  Infrared absorption, 88  
  Raman scattering, 94  
Internal coordinate, 46, 59  
Internal symmetry coordinate, 108  
Internal tension, 73  
Inverse polarization (*ip*), 94  
Inversion doubling, 176  
Irreducible representation, 37  
  Direct products of, 377  
Kronecker's delta ( $\delta_{ij}$ ), 38  
Lagrange's equation, 16  
Laser-ablated metal vapor, 112  
Laser lines, 7  
L-matrix, 85  
Lattice vibrations, 129  
Matrix algebra, 368  
Matrix co-condensation reaction, 112  
Matrix effect, 112  
Maxwell-Boltzmann distribution law, 5, 9, 97  
Metal cluster compounds, 250  
Metal isotope spectroscopy, 79, 81  
Molecular spectra, origin of, 1  
Multiplication table, 36  
Mutual exclusion rule, 34  
Nanotubes, 271  
Nitrogen compounds, 279  
Nonsymmetric vibration, 29  
Normal coordinate (*Q*), 17  
Normal coordinate analysis (NCA), 58  
**Normal modes of vibration**  
   $\text{CH}_3\text{X}$  molecule, 83  
   $\text{CH}_2\text{X}_2$  molecule, 84  
  WXYZ (bent) molecule, 192  
   $\text{X}_3$  (triangular) molecule, 170  
   $\text{X}_4$  (square-planar) molecule, 188  
   $\text{X}_4$  (tetrahedral) molecule, 187  
   $\text{XY}_2$  (bent) molecule, 30, 31  
   $\text{XY}_2$  (linear) molecule, 28, 33  
   $\text{XY}_3$  (planar) molecule, 181  
   $\text{XY}_3$  (pyramidal) molecule, 174  
   $\text{XY}_4$  (square-planar) molecule, 210  
   $\text{XY}_4$  (tetrahedral) molecule, 194  
   $\text{XY}_5$  (trigonal-bipyramidal) molecule, 214  
   $\text{XY}_6$  (octahedral) molecule, 221  
   $\text{X}_2\text{Y}_2$  (nonlinear) molecule, 189  
   $\text{X}_2\text{Y}_6$  (bridged) molecule, 241  
   $\text{X}_2\text{Y}_6$  (ethane-type) molecule, 243  
  XYZ (linear) molecule, 160  
  ZXY<sub>4</sub> (tetragonal-pyramidal) molecule, 217  
Normal vibration, 15, 18  
  number in each species, 39, 373  
Optical branch, 131  
Orbital valence force (OVF) field, 74  
Order of group (*h*), 37  
Orthogonal matrix, 108  
Overtone bands, 5, 11  
Parabolic potential, 10  
Phosphorus compounds, 285  
Plane of symmetry ( $\sigma$ ), 22  
Point groups, 23, 25~28, 355  
Polarizability, 32  
Polarizability ellipsoid, 32, 33  
Polarizability tensor, 32  
Polarized infrared spectra, 134  
Polarized Raman spectra, 134  
Potential energy curve, 10  
Potential energy distribution (PED), 87  
Potential field, 71  
Pressure broadening, 89  
Product rule, 78  
Proper rotation, 42  
Raman scattering, 6  
**Raman spectra**  
   $[\text{B}_6\text{X}_6]\text{Cs}_2$  (*X* = Cl, Br, I), 256  
   $\text{CaCO}_3$  (calcite), 136  
  Carbon nanotubes, 273  
   $\text{CCl}_4$ , 9, 93  
   $\text{C}_{60}$ , 261, 262  
   $\text{C}_{70}$ , 266  
   $\text{Eu}@C_{74}$ , 268  
   $\text{I}_2$ , 102  
   $[\text{IrCl}_6]^{2-}$ , 230  
   $\text{MF}_6$  (*M* = Mo, Tc, Ru, Rh), 230

**Raman spectra (Continued)**

- $N_2$  polymer, 158  
 $[N_5]^+[AsF_6]^-$ , 157  
 $[NO_3]K$ , 183  
 $N_4X_4$  ( $X = S, Se$ ), 285  
 $[OsF_nCl_{6-n}]^{2-}$  ( $n = 2 \sim 4$ ), 236  
 $Pb_6O(OH)_6(ClO_4)_4H_2O$ , 252  
 $P_4N_4Cl_8$ , 291  
 $Sc_2@C_{84}$ , 271  
 $Sc_3N@C_{80}$ , 270  
 $Si_n$  ( $n = 4, 6, 7$ ), 277  
 $Si_6H_{12}$ , 278  
 $SiO_2$  ( $\alpha$ -quartz), 280  
 $(SNH)_4$ , 295  
 $[SuX_3]^-$  ( $X = Cl, Br, I$ ), 178  
 $[SO_4]K_2$ , 203  
 $TiI_4$ , 103  
 $XeF_4$ , 212  
 $YBa_2Cu_3O_{7-\delta}$ , 139  
 Rayleigh scattering, 6  
 Redlich-Teller product rule, 78  
 Reduced mass ( $\mu$ ), 9  
 Reducible representation, 37  
 Redundant condition, 46  
 Representation of the group ( $\Gamma$ ), 36  
 Resonance fluorescence, 8  
 Resonance Raman scattering, 8  
**Resonance Raman (RR) spectra**  
 $I_2$ , 102  
 $Ni(OEP)$ , 105  
 $[Re_2F_8]^{2-}$ , 248  
 $TiI_4$ , 103  
**R-matrix**, 60  
 Rotational spectra, 3, 4  
 Rotational-vibrational spectrum, 232  
 Rotation-reflection axis ( $S_p$ ), 22  
  
 Salt-molecule reaction, 114  
 Schönflies (S) notation, 117  
 Schrödinger wave equation, 10, 21  
 Screw axis, 118  
 Secular equation, 75  
 Selection rules, 25, 49  
 Selenium compounds, 292  
 Silanone ( $H_2SiO$ ), 187  
 Silicates, 278  
 Silicon clusters, 276  
 Silicon compounds, 276  
 Similarity transformation, 37

- Simultaneous transition, 191  
 Site group analysis, 122  
 Site symmetry, 122, 407  
**S-matrix**, 62  
 Space group, 118, 120  
 Stokes line, 8  
 Structure determination, 56  
 Subgroup, 119  
 Sulfate radical ( $SO_4$ ), 203  
 Sulfur compounds, 292  
 Sum rule, 78  
**S vector**, 62  
 Symmetric vibration, 29  
 Symmetry coordinate, 67  
 Symmetry elements, 21, 24  
 Symmetry in crystals, 115  
 Symmetry of normal vibration, 26  
 Symmetry operation, 22  
  
 Taylor's series, 16  
 Theoretical calculation of vibrational frequencies, 106  
 Time-resolved resonance Raman (TR<sup>3</sup>) spectroscopy, 248  
 Totally symmetric vibration, 29  
 Triply degenerate vibration, 26  
 T-shaped molecules, 184  
  
 $UF_6$ , 229, 232  
**U-matrix**, 66  
 Urey-Bradley force (UBF) field, 72  
 $u$ -vibration, 34

van der Waals complexes, 159

Vibrational coupling, 84

**Vibrational frequencies**

- WXYZ molecules, 193  
 $X_2$  molecules, 150, 155  
 $X_3$  (linear, bent, triangular) molecules, 169  
 $X_4$  (tetrahedral) molecules, 188  
 $X_4$  (square-planar) molecules, 188  
 XXY (bent, linear) molecules, 170  
 XY molecules, 151, 156  
 $XY_2$  (bent, linear) molecules, 161, 164, 168  
 $XY_3$  (planar) molecules, 182, 183  
 $XY_3$  (pyramidal) molecules, 175, 177, 179  
 $XY_4$  (distorted tetrahedral) molecules, 201  
 $XY_4$  (square-planar) molecules, 211  
 $XY_4$  (tetrahedral) molecules, 194, 196, 202

- $XY_5$  (tetragonal pyramidal) molecules, 218  
 $XY_5$  (trigonal bipyramidal) molecules, 215  
 $XY_6$  (octahedral) molecules, 223, 233  
 $XY_7$  (pentagonal bipyramidal) molecules, 238  
 $X_2Y$  (linear, bent) molecules, 170  
 $X_2Y_2$  molecules, 190  
 $X_2Y_4$  molecules, 239  
 $X_2Y_6$  (ethane-type) molecules, 245  
 $X_2Y_6$  (non-planar, bridged) molecules, 242  
 $X_2Y_6$  (planar, bridged) molecules, 243  
 $X_2Y_7$  molecules, 246  
 $X_2Y_9$  molecules, 249  
 $XY_4WZ$  (octahedral) molecules, 234  
 $XYZ$  (bent) molecules, 172  
 $XYZ$  (linear) molecules, 171  
 $XY_5Z$  (octahedral) molecules, 234  
 $XY_5Z_2$  (pentagonal-bipyramidal) molecules, 238  
 $ZWXY_2$  (tetrahedral) molecules, 209  
 $ZXY_2$  (planar) molecules, 185  
 $ZXY_2$  (pyramidal) molecules, 180  
 $ZXY_3$  (tetrahedral) molecules, 205  
 $ZXY_4$  (tetragonal pyramidal) molecules, 218  
 $ZXY_4$  (trigonal bipyramidal) molecules, 215  
 $Z_2XY_2$  (tetrahedral) molecules, 207  
 $ZXYW$  (planar) molecules, 185  
Vibrational quantum number ( $\nu$ ), 11  
Water ( $H_2O$ ) molecule, 30, 33  
Water, liquid, 167  
Xenon hexafluoride ( $XeF_6$ ), 229, 231  
Xenon pentafluoride anion ( $[XeF_5]^-$ ), 57  
Xenon tetrafluoride ( $XeF_4$ ), 56  
X-matrix, 60  
Zero-point energy, 3