

# INDEX

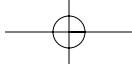
## **A**

Absorbance, 384  
 Acetals  
 infrared spectra, 52  
 Acetone-d<sub>5</sub>  
 NMR spectrum, 202  
 Acetonides, 358  
 Acetophenone  
 infrared spectrum, 59  
 mass spectrum, 477  
 Acetyl chloride  
 infrared spectrum, 72  
 Acetylacetone  
 NMR spectrum, 339  
 Acetylene  
 diamagnetic anisotropy, 129  
 (*S*)-(+)-O-Acetylmandelic acid  
 chiral resolving agent, 354  
 Acid chlorides  
 infrared spectra, basic information, 72  
 Acids  
*see Carboxylic acids*  
 Alcohols  
 effect of exchange rate, 329  
 exchange phenomena, 329  
 hydrogen-bonding effects, 48  
 infrared spectra, basic information, 47  
 mass spectral fragmentation, 464  
 NMR spectra, 329  
 NMR spectra, basic information, 149  
 Aldehydes  
 infrared spectra, basic information, 56  
 mass spectral fragmentation, 472  
 NMR spectra, basic information, 154  
 ultraviolet empirical rules, 402  
 Alkanes  
 infrared spectra, basic information, 31  
 mass spectral fragmentation, 451  
 NMR spectra, basic information, 142  
 Alkenes  
 alkyl-substituted, 38  
 C—H out-of-plane bending, 41  
*cis*-disubstituted, 42  
 infrared spectra, basic information, 33

infrared spectra, symmetrically substituted, 17  
 mass spectral fragmentation, 455  
 monosubstituted, 42  
 NMR spectra, 277  
 NMR spectra, basic information, 144  
 pseudosymmetric, 17  
 resonance effects, 39  
 ring size effects, 39  
 symmetric, 17  
*trans*-disubstituted, 42  
 Alkyl halides  
*see also Chlorides, Bromides, Iodides, and Halogen Compounds.*  
 infrared spectra, basic information, 84  
 NMR spectra, basic information, 148  
 Alkynes  
 infrared spectra, basic information, 35  
 mass spectral fragmentation, 459  
 NMR spectra, basic information, 146  
 pseudosymmetric, 17  
 symmetric, 17  
 Allenes  
 infrared spectra, 41  
 Allowed transition, 382  
 Allylic coupling, 244  
 4-Allyloxyanisole  
 NMR spectrum, 281, 290  
 alpha-cleavage, 448  
 Amides  
 infrared spectra, basic information, 70  
 mass spectral fragmentation, 488  
 NMR spectra, 345  
 NMR spectra, basic information, 159  
 restricted rotation effects, 346  
 Amine salts  
 infrared spectra, basic information, 80  
 Amines  
 infrared spectra, basic information, 74  
 mass spectral fragmentation, 484  
 NMR spectra, 340  
 NMR spectra, basic information, 152  
 pH effects on NMR spectra, 342  
 types of coupling, 342  
 Amino acids  
 infrared spectra, basic information, 80  
 Anethole  
 NMR spectrum, 290  
 Anhydrides  
 infrared spectroscopy, basic information, 73  
*p*-Anisic acid  
 mass spectrum, 483  
 Anisole  
 infrared spectrum, 51  
 NMR spectrum, 287  
 Anisotropy, 112, 128  
 Answers to selected problems, ANS-1  
 Anthracene  
 ultraviolet spectrum, 409  
 Aromatic compounds  
 NMR spectra, basic information, 145  
 NMR spectroscopy, 285  
 ultraviolet spectra, 402  
 Aromatic hydrocarbons  
 mass spectral fragmentation, 459  
 Aromatic rings  
 C—H out-of-plane bending, 45  
 infrared spectra, aromatic bands, 46  
 infrared spectra, basic information, 43  
 substitution patterns, infrared, 46  
 substitution patterns, NMR, 285  
 Aryl halides  
 infrared spectra, basic information, 84  
 Asymmetric stretch, 18  
 Attached proton test (APT), 598  
 Autobaseline, 86  
 Auxochrome, 389

## **B**

Background spectrum, 25, 86  
 Base peak, 436  
 Bathochromic shift, 389  
 Beer-Lambert Law, 383



## I-2 Index

- Benzaldehyde  
infrared spectrum, 57  
mass spectrum, 474  
NMR spectrum, 289
- Benzene  
diamagnetic anisotropy, 128  
mass spectrum, 460  
ring current, 128  
ultraviolet spectrum, 404
- Benzene derivatives  
coupling constants, 291  
NMR spectroscopy, 285  
*ortho*-hydrogens, 288  
*para*-disubstituted rings, 288
- Benzenesulfonamide  
infrared spectrum, 83
- Benzenesulfonyl chloride  
infrared spectrum, 83
- Benzene-thiol  
infrared spectrum, 81
- Benzoic acid  
infrared spectrum, 63  
ultraviolet spectrum, 385
- Benzonitrile  
infrared spectrum, 78  
mass spectrum, 490
- Benzoyl chloride  
infrared spectrum, 72
- Benzoyl derivatives  
ultraviolet empirical rules, 408
- Benzyl acetate  
NMR spectrum, 122, 123
- Benzyl alcohol  
mass spectrum, 468
- Benzyl isocyanate  
infrared spectrum, 78
- Benzyl laurate  
mass spectrum, 480
- Bicyclo[2.2.1]heptane  
mass spectrum, 455
- Boltzmann distribution, 111
- Bromides  
infrared spectra, basic information, 85
- 1-Bromo-2-chloroethane  
mass spectrum, 496
- 1-Bromohexane  
mass spectrum, 492
- Bullvalene  
valence tautomerism, 338
- Butane  
mass spectrum, 451
- 2-Butanol  
infrared spectrum, 48
- 2-Butanone  
mass spectrum, 475
- Butyl butyrate  
mass spectrum, 479
- Butyl methacrylate  
mass spectrum, 424
- Butyl methyl ether  
NMR spectrum, 151
- Butylamine  
infrared spectrum, 75  
NMR spectrum, 340
- Butylbenzene  
mass spectrum, 463
- Butyramide  
NMR spectrum, 160
- Butyric acid  
mass spectrum, 483
- Butyronitrile  
infrared spectrum, 77
- Butyrophenone  
mass spectrum, 478
- C**
- Calculation of Carbon-13 chemical shifts (Appendix 8), A-22
- Calculation of proton chemical shifts (Appendix 6), A-17
- Carbon dioxide  
background spectrum, 87
- Carbon tetrachloride  
infrared spectrum, 85
- Carbon-13 NMR spectra, 177
- Carbon-13 NMR spectroscopy  
acquisition time, 189  
aromatic rings, 197  
calculation of chemical shifts, 180  
calculation of C-13 chemical shifts (Appendix 8), A-22
- carbon-13 chemical shift values (Appendix 7), A-21
- carbon-13 chemical shifts for NMR solvents (Appendix 10), A-33
- correlation chart, C-13 coupling constants (Appendix 9), A-32
- correlation chart, carbonyl and nitrile carbons, 180
- correlation table, 179
- coupling of carbon to other elements, 199–206
- coupling to deuterium, 199
- coupling to fluorine, 203
- coupling to phosphorus, 204
- cross polarization, 185, 186
- integration, 189
- n* + 1 Rule, 181
- nuclear Overhauser effect, 186
- off-resonance decoupling, 192
- proton-coupled spectrum, 182
- proton-decoupled spectrum, 183
- relaxation effects, 190
- solvents, 199
- spin-spin splitting, 181
- Carboxylate salts  
infrared spectra, basic information, 80
- Carboxylic acids  
hydrogen-bonding effects, 53, 64  
infrared spectra, basic information, 62  
mass spectral fragmentation, 482  
NMR spectra, basic information, 158  
ultraviolet empirical rules, 402
- Charge transfer, 405
- Charge-site initiated cleavage, 448
- Chemical equivalence, 120, 195, 247
- Chemical shift, 113, 123
- Chemical shift reagents, 351
- Chemical shift table, 125
- Chiral resolving agents, 354
- Chlorides  
infrared spectra, basic information, 85
- 1-Chloro-2-methylbenzene  
mass spectrum, 497
- Chloroacetamide  
NMR spectrum, 348
- 1-Chlorobutane  
NMR spectrum, 149
- 2-Chloroethanol  
NMR spectrum, 276, 334
- Chloroform  
infrared spectrum, 86
- Chloroform-*d*
- C-13 NMR spectrum, 200
- 2-Chloroheptane  
mass spectrum, 493
- $\beta$ -Chlorophenetole  
NMR spectrum, 275
- $\alpha$ -Chloro-*p*-xylene  
NMR spectrum, 146
- Chromophore, 387
- CI-MS, 421
- trans*-Cinnamic acid  
NMR spectrum, 278
- Citric acid  
NMR spectrum, 257
- Citronellol  
C-13 NMR spectrum, 596  
COSY spectrum, 607  
DEPT spectrum, 597
- Color, 412
- Combination band, 19
- Combined structure problems, 520
- Combustion analysis, 2
- Common multiple bond systems  
diamagnetic anisotropy, 130
- Complex multiplets, 264
- Conjugation effects, *see Resonance effects*
- Cope rearrangements, 339
- Correlation chart  
C-13 NMR chemical shifts, 178  
common ultraviolet chromophores, 390

- infrared absorption frequencies, 29  
 infrared absorption frequencies  
     (Appendix 1), A-2  
 NMR chemical shift values, 124  
 NMR coupling constants, 140  
 NMR proton chemical shift values  
     (Appendix 3), A-9  
 NMR proton coupling constants  
     (Appendix 5), A-13  
 Correlation table  
     carbon-13 NMR spectroscopy, 179  
     proton chemical shift values, 125  
     COSY technique, 602ff.  
 Coupling  
     long-range, 244  
     one-bond,  $^1J$ , 235  
     two-bond,  $^2J$ , 236  
 Coupling constant, 138, 234–247  
     alkenes, 277  
     allylic coupling,  $^4J$ , 244, 280  
     aromatic rings, 291  
     benzene derivatives, 291  
     dependence on HCH bond angle, 237  
     homoallylic coupling,  $^5J$ , 245  
     long range coupling, 244  
     measuring first-order spectra, 260  
     symbols, 233  
     variation with dihedral angle, 241  
 W-coupling,  $^4J$ , 246  
*para*-Cresol  
     infrared spectrum, 48  
 Cross polarization, 185  
 Crotonaldehyde  
     infrared spectrum, 57  
 Crotonic acid  
     NMR spectrum, 280  
 Cycloalkanes  
     mass spectral fragmentation, 454  
 Cyclohexane  
     infrared spectrum, 33  
 Cyclohexanol  
     C-13 NMR spectrum, 196  
     mass spectrum, 468  
 Cyclohexanone  
     C-13 NMR spectrum, 197  
     mass spectrum, 476  
 Cyclohexene  
     C-13 NMR spectrum, 196  
     infrared spectrum, 34  
 Cyclopentane  
     mass spectrum, 454  
 Cyclopentanone  
     infrared spectrum, 60
- D**
- Decane  
     infrared spectrum, 32  
 Decoupling, 183  
     off-resonance, 192  
 DEPT, 192
- DEPT technique, 595  
 DEPT-135, 194  
 DEPT-45, 194  
 DEPT-90, 194  
 Deshielding, 129  
 Desorption ionization  
     matrix compounds, 426–427  
 Determining absolute configuration  
     *via* NMR, 356  
 Determining relative configuration  
     *via* NMR, 356, 358  
 Deuterium  
     coupling to carbon-13, 199  
 Deuterium exchange, 333  
 Deuterium labeling, 335  
 DI, 425  
 Diamagnetic anisotropy, 112, 128  
 Diamagnetic shielding, 112, 124  
 Diastereotopic groups, 252  
 Dibromomethane  
     mass spectrum, 495  
 Dibutyl ether  
     infrared spectrum, 51  
 Dibutylamine  
     infrared spectrum, 75  
 1,2-Dichlorobenzene  
     C-13 NMR spectrum, 199  
 1,3-Dichlorobenzene  
     C-13 NMR spectrum, 199  
 1,4-Dichlorobenzene  
     C-13 NMR spectrum, 199  
 Dichloromethane  
     mass spectrum, 495  
 Dienes  
     ultraviolet empirical rules, 394  
 Diethyl succinate  
     NMR spectrum, 274  
 Diethylamine  
     mass spectrum, 485  
*meta*-Diethylbenzene  
     infrared spectrum, 44  
*ortho*-Diethylbenzene  
     infrared spectrum, 44  
*para*-Diethylbenzene  
     infrared spectrum, 44  
 Difference band, 19  
 Dihedral angle, 241  
 Diisopropyl ether  
     mass spectrum, 470  
 Diketones, 61  
     Dimethyl methylphosphonate  
         C-13 NMR spectrum, 205  
 2,2-Dimethylbutane  
     C-13 NMR spectrum, 195  
*N,N*-Dimethylformamide  
     NMR spectrum, 347  
 Dimethylpolyenes  
     ultraviolet spectra, 390  
 Dimethylsulfoxide-d<sub>6</sub>  
     C-13 NMR spectrum, 200
- 2,4-Dinitroanisole  
     NMR spectrum, 291  
 Diode-array spectrophotometer, 384  
 Di-*sec*-butyl ether  
     mass spectrum, 471  
 Distortionless Enhancement by  
     Polarization  
     Transfer, *see DEPT*  
 Dopamine  
     mass spectrum, 436  
 Downfield, 115  
 Dynamic NMR, 338
- E**
- EI-MS, 420  
 Electromagnetic spectrum, 15  
 Electron multiplier, 435  
 Electronegativity effects  
     infrared, C=O stretch, 55  
     NMR diamagnetic shielding, 124  
 Elemental analysis  
     determination of carbon, 1  
     determination of hydrogen, 1  
 Empirical formula, 2  
 Enantiotopic groups, 251  
 Enones  
     ultraviolet empirical rules, 400  
 Epoxides  
     infrared spectra, 52  
 Equivalent hydrogens, 120  
 ESI, 426  
 Esters  
     infrared spectra, basic information, 64  
     mass spectral fragmentation, 477  
     NMR spectra, basic information, 157  
     resonance effects, 67  
     ring size effects (in lactones), 68  
     ultraviolet empirical rules, 402  
 Ethanol  
     NMR spectrum, 331, 332  
 Ethers  
     infrared spectra, basic information, 50  
     mass spectral fragmentation, 470  
     NMR spectra, basic information, 151  
 Ethyl 2-methyl-4-pentenoate  
     NMR spectra in various solvents, 350  
 Ethyl 3-aminobenzoate  
     infrared spectrum, 526  
     NMR spectrum, 526  
 Ethyl bromide  
     mass spectrum, 494  
 Ethyl butyrate  
     infrared spectrum, 65  
 Ethyl chloride  
     mass spectrum, 494

## I-4 Index

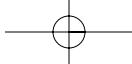
- Ethyl crotonate  
 C-13 NMR spectrum, 618  
 COSY spectrum, 621  
 DEPT spectrum, 618  
 HETCOR spectrum, 622  
 Infrared spectrum, 617  
 NMR spectrum, 620
- Ethyl cyanoacetate  
 C-13 NMR spectrum, 529  
 infrared spectrum, 529  
 NMR spectrum, 529
- Ethyl iodide  
 NMR spectrum, 132  
 NMR splitting analysis, 136
- Ethyl methacrylate  
 NMR spectrum, 361  
 NOE difference spectrum, 361
- Ethyl phenylacetate  
 C-13 NMR spectrum, 182
- Ethyl propionate  
 C-13 NMR spectrum, 523  
 infrared spectrum, 522  
 mass spectrum, 522  
 NMR spectrum, 523
- 2-Ethyl-2-methyl-1,3-dioxolane  
 mass spectrum, 471
- Ethylamine  
 mass spectrum, 485
- Ethylbenzene  
 NMR spectrum, 287
- Ethylmalonic acid  
 NMR spectrum, 159
- N-Ethynicotinamide  
 NMR spectrum, 345
- Even-electron rule, 447
- Exact mass  
 use of, 12
- Excess population  
 nuclear spin states, 111
- Extinction coefficient, 384
- Extracting coupling constants  
 systematic method, 266
- F**
- FAB, 425  
 Fast atom bombardment, 425  
 Fermi resonance, 19, 73  
 Field map, 594  
 First-order spectra, 268  
 Fluorides  
 infrared spectra, basic information, 85  
 Forbidden transitions, 382  
 Force constant, 20  
 Fourier transform, 25, 118  
 Fragment ion, 438  
 Fragmentation patterns, 445*ff.*  
 Free-induction decay (FID), 117, 593  
 Frequency domain, 116, 118  
 Frequency domain spectrum, 25  
 Frequency-wavelength conversions, 16
- FT-IR, 25  
 FT-NMR, 116  
 Fundamental vibration, 19  
 Furans  
 coupling, 293  
 Furfuryl alcohol  
 NMR spectrum, 295
- G**
- Gas chromatograph-mass spectrometer (GC-MS), 431  
 Geminal coupling, 236  
 Graphical analysis, *see Tree diagrams*  
 Gyromagnetic ratio, *see Magnetogyric ratio*
- H**
- $\alpha$ -Haloesters, 69  
 Halogen compounds  
 isotope ratio patterns, 445  
 mass spectral fragmentation, 492  
 $\alpha$ -Haloketones, 62  
 HETCOR technique, 602, 608  
 Heteroaromatic systems, 293  
 Heteronuclear, 181  
 Heteronuclear coupling, 233  
 Heteronuclear multiple-quantum correlation, 613  
 Heteronuclear single-quantum correlation, 613  
 Hexanenitrile  
 mass spectrum, 489  
 1-Hexanol  
 infrared spectrum, 47  
 NMR spectrum, 353  
 NMR spectrum, with shift reagent, 353  
 1-Hexene  
 infrared spectrum, 34  
 High performance liquid chromatography-mass spectrometry, 420  
 HMQC, 613  
 Homallylic coupling, 245  
 Homonuclear, 181, 233  
 Homopropargylic coupling, 245  
 Homotopic groups, 250  
 Hooke's Law, 20  
 HPLC-MS, 420  
 HSQC, 613  
 Hybridization effects  
 infrared, C—H stretch, 36  
 infrared, force constants, 20  
 NMR, 126  
 Hydrogen bonding effects  
 infrared, alcohols and phenols, 48  
 infrared, C=O stretch, 53, 56, 62, 68  
 NMR, 127  
 Hydrogen deficiency, 6
- Hyperchromic effect, 389  
 Hypochromic effect  
 common ultraviolet chromophores, 389  
 Hypsochromic shift, 389
- I**
- Imines  
 infrared spectra, basic information, 77  
 Index of hydrogen deficiency, 6, 7  
 Index of spectra (Appendix 14), A-46  
 Inductive cleavage, 448  
 Infrared spectrophotometer  
 dispersive, 23, 24  
 Fourier transform, 24, 25  
 Infrared spectroscopy, 15  
*See also individual functional group entries*  
 alkenes, *cis*-disubstituted, 42  
 alkenes, monosubstituted, 42  
 alkenes, *trans*-disubstituted, 42  
 alkyl-substituted alkenes, 38  
 base values, 30  
 C≡C stretch, 35  
 C≡N stretch, 78  
 C=C stretch, resonance effects, 21  
 C=C stretch, ring size effects, 39  
 C=N stretch, 78  
 C=O stretch, base values, 53  
 C—H bending, alkenes, out-of-plane, 42  
 C—H bending, aromatic, out-of-plane, 45  
 C—H bending, isopropyl, 38  
 C—H bending, methyl and methylene, 38  
 C—H bending, *tert*-butyl, 38  
 C—H stretch, 36  
 C—O stretch, alcohols and phenols, 49  
 C—O stretch, ethers, 51  
 combination and overtone bands, aromatic rings, 46  
 correlation chart, 28  
 correlation chart (Appendix 1), A-2  
 dipole moment, 16  
 functional group absorption frequencies (Appendix 1), A-2  
 general approach to analysis, 30  
 N=O stretch, 80  
 N—H bending, 72, 76  
 N—H stretch, 71, 76, 80, 82  
 O—H stretch, alcohols and phenols, 48  
 S=O stretch, 81  
 S—O stretch, 82

- Infrared spectrum, 26  
 Infrared-active, 18  
 Infrared-inactive, 18  
 In-plane vibration, 18  
 Integration, 189  
 Interferogram, 25  
 Inverse detection methods, 612  
 Iodides  
     infrared spectra, basic information, 85  
 Ion trap, 431  
 Ionization methods  
     chemical ionization, 421  
     chemical ionization reagent gases, 422  
     desorption ionization, 425  
     electron ionization, 420  
     electrospray ionization, 426  
     thermospray ionization, 426  
 Ionization potential, 420  
 $\alpha$ -Ionone  
     mass spectrum, 458  
 $\beta$ -Ionone  
     mass spectrum, 458  
*ipso*-Carbon, 180  
 Isobutane  
     mass spectrum, 452  
 Isobutyl acetate  
     NMR spectrum, 157  
 Isobutyl salicylate  
     mass spectrum, 482  
 Isobutyric acid  
     infrared spectrum, 63  
 Isochronous, 248  
 Isocyanates  
     infrared spectra, basic information, 77  
 Isopentyl acetate  
     COSY spectrum, 606  
     DEPT spectrum, 194, 595  
     HETCOR spectrum, 610  
 Isopropylbenzene  
     mass spectrum, 462  
 Isoquinoline  
     ultraviolet spectrum, 410  
 Isothiocyanates  
     infrared spectra, basic information, 77  
 Isotope ratio data, 443  
 Isotopes  
     natural abundances, 443  
     precise masses, 441
- K**  
 Karplus relationship, 241  
 KBr pellet, 26  
 Ketals  
     infrared spectra, 52  
 Ketenes, 61  
 Keto-enol tautomerism, 338  
 Ketoesters, 69
- Ketones  
     infrared spectra, basic information, 58  
     mass spectral fragmentation, 473  
     NMR spectra, basic information, 156  
     resonance effects, 60  
     ring size effects, 61
- L**  
 Laboratory frame of reference, 590  
 Lactams  
     infrared spectra, 71  
 Lactones  
     infrared spectra, 68  
 Lanthanide shift reagents, 352  
 Larmor frequency, 110  
 Lavandulyl acetate  
     mass spectrum, 423  
 Leucine  
     infrared spectrum, 81  
 Limonene  
     mass spectrum, 457  
 Lysozyme  
     mass spectrum, 428
- M**  
 Magnetic anisotropy, 128  
 Magnetic equivalence, 247, 248  
 Magnetic resonance imaging (MRI), 614  
 Magnetogyric ratio, 108  
 MALDI, 425  
 Mass analysis, 429  
     double-focusing mass spectrometer, 430  
     magnetic sector, 429  
     quadrupole ion trap, 431  
     quadrupole mass analyzer, 430  
     time-of-flight, 432  
 Mass analyzer, 429  
 Mass spectrometer, 418  
     data system, 419  
     detector, 418  
     ion source, 418  
     mass analyzer, 418  
     sample inlet, 418  
 Mass spectrometry (*incl. Appendix 11*), 12, 418, A-34  
     1,2-elimination, 466  
     1,4-elimination, 466  
      $\alpha$ -cleavage 448, 472, 448  
     base peak, 436  
     basic equations, 429  
      $\beta$ -cleavage, 473  
     chemical ionization, 421  
     common fragment ions  
         (Appendix 12), A-40  
     computer matching of spectra, 497  
     dehydration, 465  
     detection, 435  
     direct probe, 419
- fragmentation patterns, 445ff.  
 ionization methods, 420  
 isotopic abundance ratios  
     (Appendix 11), A-34  
 M+1, M+2 peaks, 438, 443  
 mass spectral fragmentation patterns  
     (Appendix 13), A-43  
 metastable ion peak, 438  
 molecular ion, 436  
 quadrupole mass analyzer, 430  
 resolution, 430  
 sample introduction, 419  
 spectral libraries, 497  
 Mass-to-charge ratio, 418  
 Matrix-assisted laser desorption ionization, 425  
 McLafferty +1 rearrangement, 479  
 McLafferty rearrangement, 450, 477, 479, 482, 488, 489  
 Measuring coupling constants from first-order spectra, 260  
 Mercaptans  
     infrared spectra, basic information, 81  
 Mesityl oxide  
     infrared spectrum, 59  
 Metastable ion peak, 438  
 2-Methoxyphenylacetic acid (MPA), 355  
 4-Methoxyphenylacetone  
     infrared spectrum, 524  
     NMR spectrum, 524  
 Methoxytrifluoromethylphenylacetic acid (MTPA), 357  
 Methyl benzoate  
     infrared spectrum, 66  
     mass spectrum, 481  
 Methyl butyrate  
     mass spectrum, 478  
 Methyl dodecanoate  
     mass spectrum, 433  
 Methyl methacrylate  
     infrared spectrum, 65  
 Methyl p-toluenesulfonate  
     infrared spectrum, 83  
 Methyl salicylate  
     infrared spectrum, 66  
 3-Methyl-2-butanol  
     infrared spectrum, 27  
 2-Methyl-1-pentene  
     NMR spectrum, 145  
 2-Methyl-1-propanol  
     NMR spectrum, 150  
 2-Methyl-2-butanol  
     mass spectrum, 466  
 5-Methyl-2-hexanone  
     NMR spectrum, 156  
 4-Methyl-2-pentanol  
     C-13 NMR spectrum, 253  
     HETCOR spectrum, 611  
     NMR spectrum, 254, 255

## I-6 Index

- N*-methylacetamide  
 infrared spectrum, 71  
*N*-Methylaniline  
 infrared spectrum, 76  
 9-Methylanthracene  
 ultraviolet spectrum, 411  
 Methylcyclopentane  
 mass spectrum, 455  
 4-Methylphenetole  
 mass spectrum, 472  
 2-Methylphenol  
 mass spectrum, 469  
 2-Methylpropanal  
 NMR spectrum, 155  
 2-Methylpyridine  
 NMR spectrum, 296  
 3-Methylpyridine  
 mass spectrum, 487  
 Microanalysis  
 accepted range, 3  
 forms, 4  
 Micrometer, 16  
 Micron, 15  
 Mineral oil  
 infrared spectrum, 32  
 Molar absorptivity, 384  
 Molecular formula, 5  
 isotope ratio method, 441  
 Molecular ion, 12, 436  
 Molecular leak, 419  
 Molecular mass determination, 5  
 Molecular weight determination  
 mass spectrometry, 12, 438  
 Mosher's method, 357  
 MPA, 355  
 MTPA, 357
- N**
- $n + 1$  Rule, 131, 181, 200, 262  
 Naphthalene  
 ultraviolet spectrum, 409  
 Neat spectrum, 26  
 Nielsen's rules, 402  
 90-degree Pulse, 591  
 Nitriles  
 infrared spectra, basic information, 77  
 mass spectral fragmentation, 488  
 NMR spectra, basic information, 153  
 Nitro compounds  
 infrared spectra, basic information, 79  
 mass spectral fragmentation, 489  
 Nitroalkanes  
 NMR spectra, basic information, 160  
 2-Nitroaniline  
 NMR spectrum, 292  
 3-Nitroaniline  
 NMR spectrum, 292  
 4-Nitroaniline  
 NMR spectrum, 292
- Nitrobenzene  
 infrared spectrum, 79  
 mass spectrum, 491  
 3-Nitrobenzoic acid  
 NMR spectrum, 294  
 1-Nitrobutane  
 NMR spectrum, 161  
 Nitrogen Rule, 12, 439  
 1-Nitrohexane  
 infrared spectrum, 79  
 2-Nitrophenol  
 NMR spectrum, 293  
 1-Nitropropane  
 mass spectrum, 490  
 NMR spectrum, 142  
 2-Nitropropane  
 COSY spectrum, 605  
 HETCOR spectrum, 609  
 NMR spectrum, 133  
 NMR spectrometer, 114  
 continuous-wave (CW), 114  
 pulsed-Fourier-transform (FT), 116  
 NMR spectroscopy, 105  
 $A_2B_2$  patterns, 270  
 $A_2X_2$  patterns, 270  
 $AA'BB'$  pattern, 290  
 AB patterns, 270  
 $AB_2$  patterns, 270  
 AMX patterns, 269  
 AX patterns, 270  
 $AX_2$  patterns, 270  
 acetonides, 358  
 acquisition time, 587  
 advanced NMR techniques, 587  
 aromatic compounds, 285  
 attached proton test (APT), 598  
 basic concepts, 105  
 bulk magnetization vector, 590  
 calculation of proton chemical shifts (Appendix 6), A-17  
 chemical equivalence, 120  
 chemical shift ranges (Appendix 2), A-8  
 chemical shift table, 125  
 chemical shifts of selected heterocyclic and polycyclic aromatic compounds (Appendix 4), A-12  
 chiral resolving agents, 354  
 common splitting patterns, 134  
 correlation chart, C-13 NMR chemical shifts, 178  
 correlation chart, chemical shift values, 124  
 correlation chart, coupling constants, 140  
 correlation chart, proton chemical shift values (Appendix 3), A-9  
 correlation chart, proton coupling constants (Appendix 5), A-13  
 correlation table, 125
- COSY technique, 602  
 coupling constants, 138, 234  
 coupling in benzene derivatives, 291  
 deceptively simple spectra, 273  
 delta, definition, 113  
 DEPT technique, 595  
 deshielding, 115  
 diamagnetic anisotropy, 112  
 diamagnetic shielding, 124  
 diastereotopic groups, 252  
 downfield, 115  
 dynamic NMR, 338  
 effect of solvent on chemical shift, 347  
 enantiotopic groups, 251  
 exchangeable hydrogens, 127  
 first-order spectra, 268  
 free induction decay (FID), 593  
 furan coupling constants, 293  
 gated decoupling, 587  
 geminal coupling, 236  
 HETCOR technique, 602, 608  
 high-field spectra, 141, 272, 351  
 homotopic groups, 250  
 integration, 121  
 intensity ratios of multiplets, 137  
 inverse detection methods, 612  
 inverse-gated decoupling, 588  
 J value, 138  
 laboratory frame of reference, 590  
 lanthanide shift reagents, 352  
 long range coupling, 244  
 magnetic equivalence, 247  
 measuring coupling constants in allylic systems, 281  
 mechanism of absorption, 109  
 mechanism of coupling, 280  
 $n + 1$  rule, 131, 262  
 90-degree pulse, 591  
 NOE-enhanced proton-coupled spectrum, 587  
 NOESY technique, 613  
 nuclear magnetization vector, 590  
 180-degree pulse, 591  
 other topics in one-dimensional NMR, 329  
 para-disubstituted aromatic rings, 288  
 phase coherence, 592  
 proton chemical shifts for NMR solvents (Appendix 10), A-33  
 proton chemical shift values (Appendix 3), A-9  
 proton coupling constants (Appendix 5), A-13  
 pulse sequences, 587  
 pulse widths, 589  
 quadrupole broadening, 342  
 quadrupole moment, 342  
 relaxation delay, 587

- resonance, definition, 110  
 rotating frame of reference, 590  
 second order spectra, 268  
 shielding, 112  
 simulation of spectra, 272  
 spin-spin coupling, 233  
 spin-spin splitting, 131, 134  
 stationary frame of reference, 590  
 two-dimensional methods  
     (2D-NMR), 602  
 upfield, 115  
 vicinal coupling, 239
- NOE**  
*see Nuclear Overhauser enhancement*  
 NOE Difference Spectra, 359  
 NOESY technique, 613  
 Nonanal  
     infrared spectrum, 57  
 Nuclear magnetic moments, 106  
 Nuclear magnetic resonance  
     *see NMR spectroscopy or C-13 NMR spectroscopy*  
 Nuclear Overhauser effect, 186  
 Nuclear Overhauser enhancement (NOE), 184  
 Nuclear Overhauser Enhancement Spectroscopy, 613  
 Nuclear spin states, 105  
 Nujol  
     infrared spectrum, 32  
 Nujol mull, 26
- O**  
 Octane  
     mass spectrum, 452  
     NMR spectrum, 143  
 2-Octanone  
     mass spectrum, 475  
 1-Octyne  
     infrared spectrum, 35  
 4-Octyne  
     infrared spectrum, 36  
 Off-resonance decoupling, 192  
 180-degree Pulse, 591  
 oop  
     *see Out-of-plane bending*  
 Optical density, 384  
 Out-of-plane bending, 42, 45  
 Out-of-plane vibration, 18  
 Overtone band, 19  
 Oximes, 78
- P**  
 Pascal's triangle, 137  
 Peak broadening  
     owing to exchange, 337  
 Peak characteristics  
     infrared spectroscopy, 27  
 2,4-Pentanedione  
     infrared spectrum, 60
- 3-Pentanol  
     mass spectrum, 465  
 1-Pentanol  
     mass spectrum, 464  
 2-Pentanol  
     mass spectrum, 465  
 (*E*)-2-Pentene  
     mass spectrum, 457  
 (*Z*)-2-Pentene  
     mass spectrum, 456  
 1-Pentene  
     mass spectrum, 456  
*cis*-2-Pentene  
     infrared spectrum, 34  
*trans*-2-Pentene  
     infrared spectrum, 35  
 1-Pentyne  
     mass spectrum, 459  
     NMR spectrum, 148  
 2-Pentyne  
     mass spectrum, 460  
 Percent transmittance, 24  
 Percentage composition, 1  
 Phase coherence, 190, 592  
 Phenol  
     mass spectrum, 469  
     ultraviolet spectrum, 386  
 Phenols  
     hydrogen bonding effects, 48  
     infrared spectra, 47  
     mass spectral fragmentation, 464  
 2-Phenyl-4-penten-2-ol  
     NMR spectra in various solvents, 349  
 Phenylacetone  
     NMR spectrum, 115  
 Phenylethyl acetate  
     NMR spectrum, 274  
 1-Phenylethylamine  
     NMR spectrum, 341  
     NMR spectrum with chiral shift reagent, 355  
 Phosphate esters  
     infrared spectra, basic information, 84  
 Phosphine oxides  
     infrared spectra, basic information, 84  
 Phosphines  
     infrared spectra, basic information, 84  
 Phosphorus compounds  
     infrared spectra, basic information, 84  
 2-Picoline  
     NMR spectrum, 296  
 Pople notation, 269  
 Population densities  
     nuclear spin states, 111  
 Precise mass  
     use of, 12  
 Precise masses of the elements, 442
- Problem solving strategy  
 NMR spectroscopy, 206  
 combined 1D- and 2D-NMR, 616  
 Prochiral, 252  
 Prochiral groups, 252  
 1-Propanol  
     C-13 NMR spectrum (off-resonance decoupled), 193  
     C-13 NMR spectrum (proton decoupled), 184  
 Propargylic coupling, 245  
 Propionamide  
     infrared spectrum, 70  
 Propionic anhydride  
     infrared spectrum, 74  
 Propylamine  
     NMR spectrum, 153  
 Proton exchange, 332  
     tautomerism, 338  
 Pulse, 116  
 Pulse sequence, 189, 587  
 Pulse width, 589, 591  
 Pulsed field gradients, 593  
 Pyridine  
     ultraviolet spectrum, 410  
 Pyridines  
     coupling, 294  
 Pyrrole  
     NMR spectrum, 344
- Q**  
 Quadrupole broadening, 342  
 Quadrupole mass spectrometer, 430  
 Quadrupole moment, 342  
 Quinoline  
     ultraviolet spectrum, 410
- R**  
 Radical-cation, 436  
 Radical-site initiated cleavage, 448  
 Reduced mass, 20  
 Relaxation, 116, 190  
 Relaxation processes, 190, 593  
 Resonance effects  
     infrared, C=C stretch, 39  
     infrared, C=O stretch, 54, 60, 74  
     infrared, ethers, 52  
     infrared, force constants, 21  
     ultraviolet, 391  
     ultraviolet, alkenes and polyenes, 391  
     ultraviolet, aromatic compounds, 406  
     ultraviolet, enones, 397  
 Retro-Diels-Alder fragmentation, 450  
 Ring current, 128  
 Ring size effects  
     alkenes, 39  
     infrared, C=C stretch, 39  
     infrared, C=O stretch, 55, 61, 68, 71



## I-8 Index

Ringing, 116  
 Rocking vibration, 18  
 Rotating frame of reference, 590  
 Rule of Thirteen, 9

**S**  
 Salt plates, 26  
 Sample preparation  
     infrared spectroscopy, 26  
 Saturation, 111  
 Scissoring vibration, 18  
 Secondary ion mass spectrometry, 425  
 Second-order spectra  
     NMR, 268  
 Shielding, 115, 129  
 Shimming, 593  
 Signal-to-noise ratio, 120  
 SIMS, 425  
 Solvent cut-offs, 386  
 Solvent shifts  
     ultraviolet, 387  
 Solvent-induced shift, 348  
 Solvents  
     effect on chemical shift, 347  
     infrared spectroscopy, 26  
 Spin system notation, 269  
 Spin-lattice relaxation, 190  
 Spin-spin relaxation, 190  
 Spin-spin splitting, 131, 134  
 Stationary frame of reference, 590  
 Stevenson's Rule, 446  
 Styrene  
     infrared spectrum, 45  
 Styrene oxide  
     NMR spectrum, 258  
 Sulfides  
     infrared spectra, basic information, 81  
 Sulfonamides  
     infrared spectra, basic information, 82  
 Sulfonates  
     infrared spectra, basic information, 82  
 Sulfones  
     infrared spectra, basic information, 82  
 Sulfonic acids  
     infrared spectra, basic information, 82

Sulfonyl chlorides  
     infrared spectra, basic information, 82  
 Sulfoxides  
     infrared spectra, basic information, 81  
 Sulfur compounds  
     infrared spectra, basic information, 81  
 Symmetric stretch, 18

**T**  
 Tautomerism  
     keto-enol, 338  
     valence, 338  
 Tesla, 108  
 Tetramethylphosphonium  
     chloride  
     C-13 NMR spectrum, 205  
 Tetramethylsilane (TMS), 113  
 Thioethers  
     mass spectral fragmentation, 491  
 Thiols  
     mass spectral fragmentation, 491  
 Time domain, 117  
 Time domain spectrum, 25  
 Tip angle, 591  
 Toluene  
     C-13 NMR spectrum, 198  
     infrared spectrum, 43  
     mass spectrum, 461  
 Tree diagrams, 257, 259  
 Tribromofluoromethane  
     C-13 NMR spectrum, 203  
 Tributylamine  
     infrared spectrum, 75  
 1,1,2-Trichloroethane  
     NMR spectrum, 131  
 Triethylamine  
     mass spectrum, 486  
 2,2,2-Trifluoroethanol  
     C-13 NMR spectrum, 204  
 2,2,4-Trimethylpentane  
     mass spectrum, 453  
 Tropylium ion, 462  
 TSI, 426  
 Twisting vibration, 18  
 Two-dimensional NMR techniques  
     (2D-NMR), 602

**U**  
 Ultraviolet spectroscopy, 381  
     band structure, 383  
     charge transfer, 405  
     conformation effects, 395  
     correlation chart, common ultraviolet chromophores, 390  
     forbidden transitions, 382  
     instrumentation, 384  
     model compounds, 411  
     pH effects, 405  
     practical guide, 413  
     solvent cut-offs, 386  
     solvent shifts, 387  
     solvents, 386  
     substituted aromatic compounds, 407  
     types of transitions, 382, 387–389  
 Unsaturation index, 6  
 Upfield, 115

**V**  
 Valence tautomerism, 338  
 Valeraldehyde  
     mass spectrum, 473  
 Valeronitrile  
     NMR spectrum, 154  
 Vibrational infrared region, 15  
 Vicinal coupling, 239  
 Vinyl  
     *see Alkenes, monosubstituted*  
 Vinyl acetate  
     infrared spectrum, 66  
     NMR spectrum, 279  
 Visible spectra, 412

**W**  
 W coupling, 246  
 Wagging vibration, 18  
 Wavelength-frequency conversions, 16  
 Wavenumbers, 15  
 Woodward-Fieser rules, 394  
 Woodward's rules, 400

**X**  
*m*-Xylene  
     mass spectrum, 462  
*o*-Xylene  
     mass spectrum, 461

