Index

a
AA’BB’ system 57, 59  
Absorption signal 128, 187  
AB system 52–53, 86  
AB$_2$ system 54, 79  
ABX system 55–57, 86  
AMX system 55, 56, 181, 192  
Axial modulation 227  
AX system 53, 130, 134, 143, 181  
AX$_2$ system 128, 146  
AX$_3$ system 146  
Alkyl, normal long chain 60, 284, 285, 360  
Amino group NH 72–74  
Anisotropic (shielding) 30–32  
APCI (atmospheric pressure chemical ionization) 238, 314  
API (atmospheric pressure ionization) 237–238, 313–314  
APT (attached proton test) 154–156

b
BB [broadband (decoupling)] 102–103  
BIRD (bilinear rotational decoupling) 137–138, 203, 207  
Bloch-Siegert shift 64  
Boltzmann’s distribution 11, 14, 143, 145

c
CA (collision activation), see CID  
CAD (collision-activated dissociation), see CID  
Carbonyl compounds 99, 101, 112, 323, 361, 362  
Characteristic frequency 322  
Chemical equivalence (equivalent) 45–49  
Chemical imaging 343–344  
Chirp 229  
CI (chemical ionization) 234–235, 310–311, 420–421

cid (collision-induced dissociation) 246–248  
Coalescence temperature 72  
Coherence 130–132, 150, 151  
Coherence order 131, 132, 151, 152  
Coherence transfer map 131  
Coherence transfer pathway 131, 132, 150  
Combined 2D NMR spectra 208–209  
Composite pulse 197  
Conjugation effect 58, 97, 323  
COLOC [(heteronuclear shift) correlation spectroscopy via long range couplings] 172–173  
Correlation time 69, 189, 191  
COSY (correlation spectroscopy) 174–178, 434–436  
– COSY-45 182–183  
– COSYLR 184–186  
– COSY with $\omega_2$ decouplings 183–184  
– H, C-COSY 169–172  
– H, X-COSY 173–174  
– DQF-COSY 186–187  
– MQF-COSY 187  
– phase sensitive COSY 178–182  
– RCO$\gamma$ 192–193  
Cross polarization 141, 142, 196  
CSI (chemical shift index) 407

d
DADI (direct analysis of daughter ions) 242  
Defocusing 241  
Dephase (dephasing) 148, 149, 150  
DEPT (distortionless enhancement by polarization transfer) 160–162  
Deuterium exchange 61, 122  
Diamagnetic shielding 7, 93  
Dihedral angle 40–41, 410, 413
Dispersion signal 128
DNMR (dynamic nuclear magnetic resonance) 70–72
DOSY 211–213
Double focusing 220
Double-quantum coherence 186, 187, 199
Double-quantum transition 68, 130
Double resonance 62–70
DSP (digital signal processing) 338

Effective field 13, 18, 19
EI [electron (impact) ionization] 233–234, 418–420
Electron effect 323
Electronegativity of substituent 29, 42, 93, 97, 102
Energy level diagram 9–10
Erythro- form 42, 401, 402
ESI (electrospray ionization) 237–238, 259, 313
Ethylene, mono-substituted 60

FAB (fast atom bombardment) 236, 311–312
FD (field desorption) 235
FFR (field-free region) 239–242
FI (field ionization) 235
FID (free induction decay) 20
Fingerprint region 327–328
Focal plan array detection 344
Formalism of product operators 184, 193, 198, 427–437
Fourier decomposition 22–23
Frequency domain signal 20
FT (Fourier transform) 20–22
FT-ICR/MS 228–231, 260
FT-IR 334–336
FT-NMR 18–25
FT-Raman 352–354
Functional group region 327
Fundamental frequency 319

γ-Gauche effect 94
Gated decoupling with suppresses NOE 104–105
GC-IR (gas chromatography-infrared spectroscopy) 344–346
GC-MS (gas chromatography-mass spectrometry) 252–253

Hartmann-Hahn matching 141–142, 196
Heavy atom effect 95
HETCOR (heteronuclear COSY), see H, C-COSY
Heteroaromatic ring 60, 293
Heteronuclear J-resolved spectrum 168–169
Heteronuclear RCOSY 193–195
HMBC [\(^1H\)-detected heteronuclear multiple bond coherence] 206–208
HMQC [\(^1H\)-detected heteronuclear multiple-quantum coherence] 203–204
HMQC-TOCSY 367
HOESY (heteronuclear NOE spectroscopy) 191–192
HOHAA (homonuclear Hartmann-Hahn spectroscopy) 196–198
HSQC [\(^1H\)-detected heteronuclear Single-quantum coherence] 204–205
HV method 241
Hybrid tandem MS 250
Hydrogen bonds 34, 38, 101, 324
Hydroxyl group OH 72–73, 360, 361
Hyperconjugation effect 94, 280

ICR (ion cyclotron resonance) 228–229
IKES (ion kinetic energy spectroscopy) 242
INADEQUATE (incredible nuclei enhancement by polarization transfer experiment) 198–201, 368
– for \(^1H\) 201–202
INCOS (MS library retrieval) 305–308
INEPT (insensitive nuclei enhanced by polarization transfer) 157–160, 204, 205, 208
Inverse mode 202–208
Inversion recovery 106–108
Ion trap 223–227
IR microscope 343–344
Iso-β lines 225, 226
Isotropic mixing 141–143, 196

J-modulation 135, 154
J-resolved spectrum 165–169

Karplus equation 40–41, 413
Index

I
Lamor frequency  5, 11, 12
LC-MS (liquid chromatography-mass spectrometry) 253–254
LC-NMR (liquid chromatography-nuclear magnetic resonance) 25–26
Linked scan  242–244

m
Magnetic equivalence (equivalent)  49–50, 51, 52
Magnetization  11–14, 127–159, etc.
Magnetogyric ratio  3, 63, 68, 92, 141, 142, 144, 151, 190
MALDI (matrix-assisted laser desorption/ionization) 236–237, 312–313
Mass analyzer  219–233
Mass effect  324
McLafferty rearrangement 273–274
Medium effect  62, 101
Mesomeric effect, see Resonant effect
Metastable ions  238–246
Michelson interferometer 334–335
Microscope (IR) 343
MIKES (mass-analyzed ion kinetic energy spectroscopy) 242
MS library retrieval 305–309
Multiple-quantum coherence 131, 187
Multiple-quantum spectroscopy  164

n
Newman projection  42, 47, 402
NIST  308
NOE (nuclear Overhauser effect)  67–70, 102, 104, 188–189, 414–417
NOESY (nuclear Overhauser effect spectroscopy) 188–189

o
oa-TOF (orthogonal acceleration TOF)  233
Overtone  320

p
paramagnetic shielding (or deshielding)  7, 93
PAS (photoacoustic spectroscopy) 337–339
PBM (probability-based matching) 308–309
Peak matching  262
PFG (pulsed-field gradient) 147–152
Phase cycling  132, 150, 151, 186, 199
Phase lag  338
Polarization transfer  145
Population difference  15, 144, 146
Prochirality (prochiral center)  48–49
Quadrature detection  129–130, 150, 179, 180
Quadrupole mass analyzer  221–223, 265
Quadrupole moment  2, 6
Quadrupole relaxation  73, 74, 105
Quasi-molecular ions  217, 234, 237, 238, 310–314
Raman scattering  347–350
Rapid scan  334–336
RDA (retro-Diels-Alder reaction) 274, 276
Reactive hydrogen atom  72–74
Refocus (refocusing)  133, 149, 150
Relaxation  14–17
– measurement of longitudinal relaxation time, T1 106–108
– measurement of transverse relaxation time  133–134
Rephase  149
Resonant effect  97, 323
Resonant ejection  227
Ring current effect  29, 30
RMS (reaction mass spectrometry) 421–422
ROESY (rotating frame Overhauser effect spectroscopy) 140, 189–190
Rotating frame  12
Sampling  75, 110
Scout scan  26
Selective excitation  152
Shaped pulse  152–154
Shielding constant  6–7, 93
Shift reagent  62
Single focusing  219–220
Single-quantum coherence  131, 187
Single-quantum transfer  68, 130, 164
Soft ionization  234–238, 420–421
SPI (selective polarization inversion) 143–146, 158, 160
Spin decoupling  63–67
Spin echo  132–136, 165
Spin locking  138–140, 142, 190, 196
Spinning side-bands  75
Stability diagram  222, 223, 225
Step scan  334–337
Stereo-selective reaction mass spectrometry, see RMS
Steric effect 93, 94, 324
Stevenson-Audier’s rule 281–283
Substituted phenyl ring 57–59, 97–98, 359–360
SWIFT (stored waveform inverse Fourier transform) 230
Symmetrical plan law 48–49

T
Tandem MS 248–252
– in space 248–251
– in time 251–252
Three-dimensional NMR 209–211
Three types of substituents 57–58
Threeo-form 42, 401, 402
Time domain signal 20
Time scale 70
TOCSY (total correlation spectroscopy) 143, 195

TOF (time-of-flight) 231–233, 265
TPPI (time proportional phase increment) 179
TRS (time resolved spectroscopy) 339–340
Two-dimensional IR 340–343
Two-dimensional NMR, introduction to 162–165

v
Virtual field 13

w
WET (water suppression enhanced through the $T_1$ effect) 26

z
Zero quantum transition 68, 130