

## Index

### Symbols

2,2-dimethyl-2-silapentane-5-sulfonic acid, 26  
3-(trimethylsilyl)propionic acid sodium salt, 26

$B_1$  field, 117

$J$ -resolved experiments, 368

$^1\text{H}$  chemical shifts

– hydrogen bonding, 37

– pH effects, 37

– solvent effects, 37

– temperature effects, 37

$^1\text{H}$  NMR

– anisotropy effects, 35

– chemical shifts, 34

– coupling constants, 50

– geminal coupling constants, 50

– general aspects, 33

– H,C coupling constants, 52

– H,F coupling constants, 53

– H,P coupling constants, 54

– influence of electronegativity on  
chemical shifts, 35

– shielding effects, 35

$^{13}\text{C}$ , 329

$^{15}\text{N}$ , 329

$^{19}\text{F}$ , 329

$^{31}\text{P}$ , 329

### A

acquisition time

– and digital resolution, 217

activation energy

– measurement of, 346

analog-to-digital converter, 16

anisotropy, 133

Arrhenius plot, 347

asymmetry, 133

audio filter, 215

autocorrelation function, 308

autorelaxation, 315

axiality, 133

### B

baseline correction

– in 2D spectra, 381

binding affinity, 400

Biot–Savart law, 127

Boltzmann distribution, 14, 293

### C

carbohydrates, 419

– establishing linkages, 429

– identification by NMR, 424

– identification of stereochemistry, 426

– quick identification, 430

– solvent choice, 429

– structure, 419

carbon-13, 59

chemical shift, 16

– diamagnetic contribution, 17

– electric field effects, 62

– heavy atom effects, 63

– hybridization effects, 61

– increment systems, 64

– isotropic, 133, 384

– mesomeric effects, 63

– neighbor anisotropy effects, 63

– paramagnetic compounds, 131

– steric effects, 62

– substituent effects, 61

chemical shift anisotropy, 128

–  $^{15}\text{N}$ , 129

chemical shift mapping, 395

chemical shift perturbation, 395, 397

coalescence, 337

coalescence temperature, 340

coherence, 108

– multiple quantum, 109

coherence selection, 287  
 coherence transfer, 271  
 complex, 401  
 composite pulse decoupling, 256  
 constant time, 279, 280  
 correlation function, 302  
 correlation time, 300  
 COSY, 358
 

- double quantum filtered, 284, 358
- multiplet pattern, 427
- triple quantum filtered, 285, 358

 coupling
 

- geminal, 136
- heteronuclear, 44, 284
- homonuclear, 18, 44, 279
- scalar, 134

 cross-relaxation, 315  
 cross-relaxation rate, 319, 320  
 CYCLOPS, 286

**D**

decoupling
 

- sidebands, 244

 delay, 272
 

- relaxation, 273

 density matrix, 172  
 DEPT, 276  
 detection, 355  
 diastereotopic, 40, 42, 43  
 diffusion, 403  
 diffusion coefficient, 403  
 digital filter, 215  
 digital resolution, 217  
 digitizer
 

- dynamic range, 214

 dipolar coupling
 

- solid state, 386

 DIPSI-2
 

- composite pulse decoupling, 256

 direct dipolar relaxation rate, 320  
 direct spin–spin coupling, 141  
 DNA quadruplexes, 484  
 downfield, 17  
 dwell time, 196

**E**

eigenstate, 156  
 eigenvalue, 156  
 electric field effect, 130  
 enantiotopic, 42  
 equivalence
 

- magnetic, 39

 exchange, 335, 398, 402
 

- chemical, 335

- conformational, 336
- examples, 342
- fast, 336, 338
- intermediate, 336, 340
- slow, 336, 340
- two state, 336

exchange rates
 

- measurement, 344

 excitation sculpting, 274  
 expectation value, 157  
 EXSY, 345  
 extreme narrowing, 320, 322

**F**

Fermi contact, 131, 135  
 Fermi contact interaction, 37  
 field
 

- effective, 384

 field gradients, 247  
 field-frequency lock, 192  
 FLOPSY, 257  
 folding, 204  
 Fourier transformation, 16
 

- discrete, 203

 free induction decay, 15, 195  
 furanoses, 421

**G**

GARP, 256  
 Gaussian pulses, 236  
 gradient spin echo, 403  
 gyromagnetic ratio, 95

**H**

Hamilton operator, 169  
 Hartmann–Hahn condition, 360  
 HETCOR, 280  
 heteronuclear cross-polarization, 276  
 heteronuclear nuclear Overhauser effect, 329  
 high-temperature approximation, 107  
 Hilbert space, 158  
 HMQC, 276, 280, 364  
 HN(CO)CACB, 283  
 HNCA, 284  
 HNCACB, 283  
 HOESY, 329  
 homotopic, 42  
 HSQC, 280, 364  
 hydrodynamic radius, 403  
 hydrogen bonds, 130

**I**

INADEQUATE, 367  
 indirect detection, 59  
 induced field, 132

inductive effect, 65  
 INEPT, 275, 279, 283  
 inhomogeneous broadening, 114  
 initial-rate approximation, 346  
 interaction  
 – dipolar, 304  
 inverse detection  
 – transition metals, 79  
 inverse gated, 69  
 inversion, 315  
 inversion recovery, 282, 306  
 irradiation, 274  
 isochronous, 39  
 isotope shift, 76

**J**

jump return, 275

**K**

Karplus relationship, 51, 137, 426

**L**

Lamb shift, 127  
 line broadening  
 – exchange, 339  
 linear approximation, 325  
 linear prediction, 219, 378, 379  
 Liouville space, 175  
 Liouville–von Neumann equation, 174  
 Lipari–Szabo, 307  
 lock, 192, 333  
 longitudinal relaxation  
 –  $^{13}\text{C}$  nuclei, 68  
 Lorentzian line shape, 199  
 – integral of, 201  
 – phase of, 201  
 lowering operator, 164  
 lowest unoccupied molecular orbital, 128

**M**

magic-angle spinning, 387  
 magnet, 181  
 magnetic anisotropy, 36  
 magnetic dipole moment, 13  
 magnetic quantum number, 95  
 magnetic susceptibility, 130  
 magnetism, 87  
 magnetization  
 – longitudinal, 106  
 – transverse, 106  
 magnetization transfer  
 – by isotropic mixing, 257  
 main group elements, 70  
 –  $^{15}\text{N}$ , 71

–  $^{19}\text{F}$ , 72  
 –  $^{31}\text{P}$ , 73  
 matching, 190  
 mixing, 288  
 mixing time, 324, 333  
 MLEV  
 – composite pulse decoupling, 256  
 model-free approach, 307  
 Mosher's reagent, 43  
 multiplet structure, 47

**N**

neighbor anisotropy effect, 129  
 NMR  
 – basic phenomena, 13  
 NMR timescale, 336  
 NOESY, 278, 325, 345, 401  
 – isotope edited, 400  
 – isotope filtered, 400  
 nuclear Overhauser effect, 315, 400  
 – enhancements, 323  
 – intermolecular, 396, 400  
 – kinetics of, 324  
 – multispin systems, 325  
 – rotating frame, 327  
 – steady state, 318, 321  
 – transient, 318, 324  
 – use in stereochemical analysis, 330  
 nuclear quadrupole coupling constant, 141  
 nuclear spin, 94  
 – properties of heteronuclei, 57  
 nucleic acids, 481  
 –  $^{13}\text{C}$  NMR, 489  
 –  $^{31}\text{P}$  NMR, 490  
 – assignments, 492  
 – labeling, 496  
 – sequential walk, 492  
 – structure, 482  
 – triple-resonance experiments, 496  
 nutation, 119  
 nutation frequency, 235  
 Nyquist theorem, 204

**O**

offset frequency, 116  
 order parameter, 308  
 out and back, 284  
 oversampling, 215

**P**

paramagnetic, 333  
 paramagnetic spin-orbit, 135  
 parts per million scale, 17  
 Pascal's triangle, 46

- Pauli principle, 135
  - Pauli spin matrices, 165
  - peak shape
    - E.COSY, 362
  - peaks
    - autocorrelation peaks, 352
  - peptide bond, 459
  - peptides, 457
    - $\beta$  strands, 459
    - $^1\text{H}$  NMR, 461
    - $^{13}\text{C}$  NMR, 464
    - $^{15}\text{N}$  NMR, 467
    - assignments, 469
    - hydrogen bonds, 459
    - NMR of, 461
    - NOESY walk, 472
    - nomenclature, 459
    - random coil chemical shifts, 463, 469
    - secondary structure, 459
    - structure, 458
    - structure calculation, 474
    - triple-resonance experiments, 473
  - phase coherence, 20, 108
  - phase correction, 227, 381
  - phase cycle, 284
    - number of steps in, 379
  - phase modulation, 371
  - Pirkle's reagent, 44
  - polarization operators, 164
  - polarization transfer, 275
    - INEPT, 266
  - power spectra, 229
  - presaturation, 258
  - prescan delay, 228
  - principal axis system, 133
  - processing
    - two-dimensional spectra, 380
  - protein dynamics, 306
  - proton spectra
    - solvent dependence, 441
  - pseudocontact shift, 37, 131
  - pulse, 272
    - calibration, 244
    - width, 234
  - pulse experiments, 271
  - pulse program, 285
  - pulsed field gradients, 247, 272, 286
- Q**
- quadrature detection, 286, 370
  - quadrupolar nuclei
    - transition metals, 81
  - quadrupolar relaxation, 141
    - metals, 57
  - quadrupole moment, 140
  - quench, 184
  - quintet, 46
- R**
- radiation damping, 115
  - radio frequency coils, 189
  - radio frequency field
    - inhomogeneity, 243
    - power dissipation, 242
  - radio frequency pulses, 15, 117
    - frequency shifted, 242
    - hard, 235
    - off-resonance effects, 243
    - soft or selective, 236
  - Ramachandran plot, 459
  - receiver phase, 210, 252, 285
  - Redfield trick, 211
  - reduced coupling, 136
  - reference frequency, 115
  - referencing, 25
    - direct, 25
  - relaxation, 293
    - chemical shift anisotropy, 297
    - longitudinal, 399
    - mechanism, 303
    - paramagnetic, 299
    - spin–spin rotation, 299
    - transverse, 398
  - relaxation delay, 333
  - relaxation dispersion, 310
  - relaxation interference, 309
  - relaxation reagent, 367
  - resolution, 216
    - in 2D spectra, 377
  - resolution enhancement
    - by apodization, 221
  - resonance frequency, 99
  - rhombicity, 133
  - ring current, 36
  - ring-current effect, 129
  - rising operator, 164
  - ROESY, 278, 327, 363
    - artifacts in, 363
  - rotating frame experiments, 363
  - rotor, 383
- S**
- salt, 24
  - sample spinning, 23, 187
  - sampling
    - sequential, 211
  - sampling rate, 204

- saturation, 315
  - saturation transfer, 274, 344
  - saturation transfer difference, 323, 344, 402
  - scalar coupling constants, 18, 474
  - scalar couplings
    - active, 353
    - geminal, 18
    - X,<sup>13</sup>C couplings, 64
  - scalar relaxation
    - of the second kind, 141
  - screening, 395
  - self-decoupling, 339
  - sensitivity enhancement, 288
    - by apodization, 221
  - septet, 46
  - sextet, 46
  - shaped pulses, 236
  - shift reagents, 37
    - chiral, 44
    - lanthanide, 44
  - Shigemi tubes, 367
  - shimming, 184
  - shims, 23
    - room temperature shims, 183, 184
  - signal dispersion, 17
  - signal-to-noise ratio, 27
  - solid-state NMR, 383
  - Solomon equations, 318
  - solvent effect, 130
  - solvent exchange, 33
  - solvent suppression, 257
  - spectral density, 305
  - spectral width, 196
  - spin angular momentum, 88
    - quantization of, 90
  - spin diffusion, 320, 322, 363
  - spin ensemble, 105
  - spin lock, 275, 327
  - spin precession
    - right-hand rule, 99
  - spin quantum number, 94
  - spinning sidebands
    - in liquid state, 187
  - spin–dipolar, 135
  - state vector, 158
  - Stern–Gerlach experiment, 93
  - steroids, 439
    - <sup>13</sup>C spectra, 443
    - assignments, 444
    - conformation, 440
    - nomenclature, 440
  - Stokes–Einstein, 403
  - strong coupling, 135
  - superposition, 108
  - superposition state, 157
- T**
- T1 noise, 332, 363
  - T1 relaxation, 293
  - temperature calibration, 333
  - tensor
    - chemical shift, 384
    - shielding, 132
    - trace, 384
  - three-dimensional NMR, 370
  - time domain signal, 195
  - time-proportional phase incrementation, 212
  - TOCSY, 278, 329
  - transferred nuclear Overhauser effect, 401
  - transition metal NMR, 78
  - transitions
    - double quantum, 140
    - multiple quantum, 140
    - single quantum, 140
    - zero quantum, 140
  - triple-resonance experiments, 283
  - triplet, 45
  - TROSY, 280
  - tumbling, 399
  - two-dimensional experiments
    - heteronuclear, 279
    - homonuclear, 278, 351
    - setup of, 379
  - two-dimensional NMR
    - building blocks, 354
    - diagonal peaks, 355
    - indirect dimension, 354
- U**
- upfield, 17
- V**
- variable-temperature NMR, 335
  - viscosity, 403
- W**
- WALTZ
    - composite pulse decoupling, 256
    - isotropic mixing, 257
  - weak coupling, 135
  - window multiplication
    - Lorentz-to-Gauss transformation, 225
- Z**
- zero-quantum artifacts, 326
  - zero-quantum interference peaks, 362
  - zigzag arrangement, 52