

Index

a

- A₂ system 158 ff.
 - eigenfunctions 168
 - eigenvalues 168
 - energy level diagram 161
 - oriented 560
 - relative intensities 162
 - secular determinant 160
 - transition energies 168
 - transition probabilities 168
 - variational method 160
- AA'BB' spectrum 205
 - direct analysis 666
- A₂X₂ system 55, 194, 203
- AA'XX' system 193 ff.
 - 4-bromoanisole 201
 - deceptively simple 203
 - direct analysis 198
 - eigenvalues 183
 - energy level diagram 196
 - furan 204
 - half spectrum 197
 - Hamilton matrix 195
 - 2-methylbenzotriazole 200
 - morpholine 203
 - subspectra 195, 197
 - symmetry functions 195
 - transition energies 199
- A₂B system 177, *see also* AB₂ system
- absolute value representation 285
- AB system 164
 - chemical exchange 522
 - CIDNP effect 609
 - deceptively simple 170
 - direct analysis 175
 - eigenfunctions 168
 - eigenvalues 168
 - energy level diagram 157
 - geometric solution 176
 - ratio $J/\nu_0\delta$ 176
 - spectrum 166
 - spin-polarized 609
 - transition energies 168
 - transition probabilities 168
- AB₂ system 177
 - basis functions 179, 182
 - direct analysis 180
 - eigenfunctions 179, 182
 - energy level diagram 180
 - Hamilton matrix 183
 - irreducible representation 182
 - particle spin 181
 - spectrum 178
 - subspectra 182
- AB_n system 182
- ABC system 191, 628
 - COSY cross peaks 628
- ABX system 628
 - AB part 190
 - deceptively simple 189
 - dependence on $\nu_A - \nu_B$ 192
 - E.COSY 628
 - effective Larmor frequencies 186, 628
 - passive spin 183, 628d
 - product functions 184
 - relative sign of coupling constants 190
 - solutions 187
 - subspectra 184
 - virtual coupling 190
 - X-approximation 183
 - X-part 188
- ABX₂ system 185
- ABX₃ system 185
- accumulation, of spectra 79
- acetylacetone 550
- acidic protons 37

- acquisition time 257
 acoustic ringing 446
 acrylonitrile, spectrum 57
 acyloxonium salt 547
 2-adamantanol, spectrum in the presence of
 Eu(DPM)₃ 602
 ADC, analog-digital-converter 254
 adenosine diphosphate (ADP) 642
 adenosine triphosphate (ATP) 642, 643
 adsorbed hydrocarbons, MAS 587
 alanine, spectral change with pH 93
 aldehyde proton deshielding 99
 aldehydes, unsaturated 99, 100
 alignment 565
 – degree of 566
 – in electric field 565
 – in phospholipids 565
 – in poly- γ -benzyl L-glutamate (PBLG) 567
 – tensor 566
 – and variable angle sample spinning 567
 allenes, long-range ^1H , ^1H coupling 142
 allylic ^1H , ^1H coupling 141
 allyl magnesium bromide 542
 alpha-helix 632
 ALTADENA 621
 – AX system 618
 aluminum-27, *see also heteronuclei* 468 ff.
 ammonium ion, ^{14}N NMR 51
 amine protons 37
 ammonia 525
 amplitude modulation 282
 AMXsystem 226
 analog–digital converter (ADC) 254
 analysis of spin systems, *see spectral analysis*
 149 ff.
 Anderson–Kubo–Sack theory 536, 671
 angular momentum 13, 16
 angular velocity 16
 anisotropy, chemical shift 30, 433, 571
 – diamagnetic, *see diamagnetic anisotropy*
 [18]annulene, ^1H NMR 104, 533
 annulenes 104 ff.
 – ring inversion, *see dynamic NMR*
 anthracene, ring current 103
 anti-aromatic molecules 106, 541
 anti-echo signal 325
 antimony(V) fluoride 67
 anti-phase magnetization 316
 antisymmetric wave functions 164
 aromatic compounds, ^1H data 652, 655
 – ^{13}C data 661
 aromatic ions 89, 411
 aromatic solvent induced shifts (ASIS) 121
 Arrhenius activation energy, E_a 507
 artifacts in COSY spectra 302
 ASIS (aromatic solvent induced shifts) 73
 assignment techniques, in ^{13}C NMR 381 ff.
 associated coupling 630
 association effects 72
 asymmetric carbon 219
 asymmetry parameter 586, 587
 atropic molecules 106
 aufbau principle 105
 axial shielding 96
 AX system 61, 169 ff.
 – CIDNP effect 612
 – COSY spectrum 61
 – double quantum selection 331
 – double resonance 59
 – energy level diagram 44, 168 ff.
 – eigenfunctions 168
 – eigenvalues 168
 – eigenstates 45
 – entropy polarization 612
 – first order approximation 167
 – operator basis 311
 – partially aligned 566
 – transition energies 168
 – transition probabilities 168
 – SPI experiment 358
 – SPI experiment, CHCl_3 359
 – spin echo experiment 288
- b**
 B_0 fields 33
 backbone angles, in peptides 630
 backbone assignment, sequential 633, 634
 basis functions 170
 benzene, chloroform complex 118
 – 1,2-dichloro- 76
 – ethyl, sensitivity test 78
 – disubstituted 212, 334
 – heptamethyl 546
 – hexamethyl 545
 – monsubstituted 91
 – oxide, valence tautomerism 538
 – *ortho*-disubstituted 334
 – *para*-disubstituted 334
 – partially oriented 562
 – ring current 69, 101
 – spectrum of partially oriented 562
 – spin-lattice relaxation 242
 – spin-spin coupling, ^1H , ^1H 658
 – – ^{13}C , ^1H 424, 426
 – 1,2,3-trichloro- 178
 – 1,2,4-trichloro- 183
 benzenium ion, heptamethyl- 546
 – hexamethyl- 545

- benzoxepine, ^1H spectrum 146
 - benzyl acetate 33, 41
 - benzyl alcohol 72
 - biochemistry, NMR in 625 ff.
 - biomolecules 625 ff.
 - bio NMR, nucleic acids 634 ff.
 - backbone torsion, scalar coupling 635
 - coherence pathway 635
 - COLOC experiment 636
 - ^{13}C , ^{31}P HMQC shift correlation 636
 - DNA structure 635
 - Haasnoot-Altona equation 638
 - helix structure 635
 - Karplus curves 635
 - mononucleotides 636
 - NOE-based pathway 635
 - phosphorus-31 NMR 635
 - torsional angles 634, 635
 - bio NMR, oligo- and polysaccharides 636 ff.
 - anomeric protons 638
 - chair $^1\text{C}_4$ 637
 - chair $^4\text{C}_1$ 637
 - galactose 637
 - glycoside linkage 637
 - Karplus curves 638
 - pyranose rings, chair conformation 637
 - sialyl- $\alpha(2\rightarrow6)$ lactose 637
 - stereochemistry 637
 - torsional angles 637
 - trisaccharide 637
 - bio NMR, peptides and proteins 627 ff.
 - α -helix 632
 - backbone angles, in peptides 630
 - backbone assignment, sequential 633, 634
 - – HCA(CO)N experiment 633
 - – HCACO experiment 633
 - – HNCA experiment 633
 - – HNCO experiment 633
 - – HOHAHA-HMQC experiment 633
 - β -sheet 632
 - β -turn 632
 - bovine pancreatic trypsin inhibitor (BPTI), 3D structure 632
 - BPTI, 3D structure 632
 - constraints 630
 - E.COSY (exclusive correlation spectroscopy) 628
 - – ABC system 628
 - – ABX system 628
 - – effective Larmor frequencies 628
 - – passive coupling 628
 - – pulse sequence 629
 - – three spin system, homonuclear 628
 - hairpin 632
 - Karplus curve, in peptides 631
 - peptide partial structure, NMR experiments 630
 - polypeptides, ^{13}C , ^{15}N enriched, scalar coupling 633
 - shift correlation ^{15}N , ^1H 629
 - spatial structure 630
 - transverse relaxation optimized spectroscopy, *see* TROSY
 - TROSY 629
 - – enzyme spectrum 629
 - biphenylene 112, 585
 - 2-methyl- 400
 - BIRD pulses 329
 - bis*(trimethylsilyl)mercury 49
 - bis*-methano[14]annulene, 1,6;8,13-*anti*- 109
 - bis*-methano[14]annulene, 1,6;8,13-*syn*- 109
 - bit, binary digit 255
 - Bloch equations 667
 - for chemical exchange 668
 - Bloch vector model 289, 297, 309
 - Bloch-Siegert shift 272
 - boat form 526, 637
 - blood plasma 640
 - body fluids, NMR of 640
 - Boltzmann relation 19
 - bond length 130, 132, 426
 - bond order 130, 132, 426
 - bond shifts, *see also dynamic NMR* 538 ff.
 - boron-11, *see also heteronuclei* 435 ff.
 - bovine pancreatic trypsin inhibitor (BPTI), 3D structure 632
 - BPTI, 3D structure 632
 - broadband decoupling 275 ff.
 - by CW modulation 275
 - by pulse methods 275
 - composite pulse sequences 278
 - MLEV 277
 - building blocks for pulse sequences 329
 - bullvalene, *see also dynamic NMR* 535, 537
 - butadiene-1.3 658
 - n*-butyllithium, PGSE experiment 615
 - t*-butylgroup, hindered rotation 522
- c**
- cadmium113, *see also heteronuclei* 488
 - carbanions 92
 - carbenium ions 67
 - carbocations, *see also dynamic NMR* 545
 - carbohydrates 636 ff.
 - carbon chemical shifts, *see also carbon-13 NMR* 659 ff.
 - alkenes 659
 - alkynes 661

- carbon chemical shifts, *see also carbon-13 NMR*
(*contd.*)
- aromatic compounds 661
 - benzenes, substituted 662
 - benzocycloalkanes 661
 - cycloalkanes 660
 - cycloalkenes 660
 - heterocycles 663
 - hydrocarbons 659
 - solvents 659
 - carbon-13 NMR**
 - APT, attached proton test 383
 - - delays for CH, CH₂, CH₃ group detection 384
 - assignment techniques 383 ff.
 - attached proton test (APT) 383
 - 4-*t*-butylcyclohexanone, spectrum 386
 - C60 416
 - C70 416
 - chemical shift 407, 408, 659 ff.
 - - α -effect 419
 - - aromatic ions 411 ff.
 - - β -effect 419
 - - carbocations 415
 - - charge density effect, aromatic systems 411 ff.
 - - dicyclopentaheptalene 414
 - - fullerenes 416
 - - γ -effect 419 ff.
 - - heavy atom effect 409
 - - Lamb formula 409
 - - NICS values 416
 - - non-alternant hydrocarbons 414
 - - paramagnetic term 410
 - - pH dependence in pyridine 414
 - - π electron density 411
 - - protonation 413
 - - pyrene 414
 - - Ramsay equation 410
 - - theoretical models 409 ff.
 - constant time experiment 394
 - correlation via long-range couplings (COLOC) 394
 - CW spectrum 378
 - DEPT sequence 388
 - - product operator formalism 388
 - - spectrum of longifolene 390
 - - subspectra 389
 - dicycloheptapentalene 414
 - diphenyl acetylene 407
 - empirical correlations 418
 - experimental aspects 381 ff.
 - first-order splitting 405
 - fullerene anions 417
 - fullerene, encapsulated ³He 417
 - gated decoupling 382
 - HETCOR 389
 - - pulse sequence 391
 - - spectrum of a paracyclophane 399
 - - - of 2,7-dilithionaphthalene 393
 - - - of angelica acid 398
 - - - of bis-dehydrobenzo[20]annulene 399
 - - - of tiglic acid 398
 - HETCOR COLOC 394
 - heavy atom effect 409
 - historical development 378
 - HMBC
 - - gradient enhanced 397
 - - spectrum of 3-fluorophenanthrene 397
 - HMQC 389, 394
 - - ¹³C, ²H shift correlation with BIRD pulse 396
 - - pulse sequence 391
 - - spectrum of
 - benzo[*c*]1,7-methano[12]annulene 393
 - - with single quantum A elimination by BIRD 394
 - pulse sequence 391
 - HSQC 391
 - INADEQUATE experiment, 1D ¹³C, ¹³C 398 ff.
 - - spectrum of 2-methylbiphenylene 400
 - - pulse sequence and vector diagrams 400
 - INADEQUATE experiment, 2D ¹³C, ¹³C, nicotine amide adenine dinucleotide (NAD⁺) 402
 - INEPT, refocused 387
 - inversion recovery experiment 381
 - isotope effects, deuterium induced, 1,6-indane oxide 406
 - *J*, δ spectrum, heteronuclear 401
 - - of norbornane 403
 - *J*-resolved spectrum, heteronuclear 401
 - longitudinal relaxation, measurement 381
 - magnetization modulated by CH coupling 387
 - multiplicity selection 383 ff.
 - polarization transfer experiments 387 ff.
 - - DEPT 388
 - - refocused INEPT 387
 - pyridine spectrum 378
 - receptivity 377
 - refocused INEPT 387
 - SEFT, spin echo Fourier transform 383
 - - delays for CH, CH₂, CH₃ group detection 384
 - - magnetization vector orientation 385
 - - selective excitation 403 ff.

- selective INEPT, phenylacetylene 404
- shift increments 419
- signal selection 384 ff.
- spherical aromaticity 416
- spin echo experiment 383
- spin flip method 402
- spin-lattice relaxation rates,
 - diphenylacetylene 407
- spin-lattice relaxation 428
 - - rotational barriers 429
 - - segmental motion 429
- spin-spin coupling constants 420 ff.
 - - and chemical structure 422 ff.
 - - ^{13}C , ^{13}C coupling, 1J 422 ff.
 - - - bond length dependence 422
 - - - cyclopropane 423
 - - - Fermi contact term 422
 - - - s-character 422
 - - - silacycloheptene 423
 - - - table 424
 - - ^{13}C , ^{13}C coupling, 3J , 423 ff.
 - - - π bond contribution 423
 - - - dihedral angle dependence 423
 - - - Karplus curve 423
 - - ^{13}C , ^1H coupling, 1J 424 ff.
 - - - benzocyclopropene 425
 - - - s-character dependence 424
 - - - correlation with bond length 426
 - - - correlation with HMO π -bond order 426
 - - - Karplus curve 427
 - - ^{13}C , X coupling 427
 - testosterone spectrum 380
 - T_1 measurement 381
 - two-dimensional chemical shift correlation 389 ff.
 - vitamin B₁₂ spectrum 379
 - *m*-xylene, T_1 measurement 381
 - cell metabolism 641
 - charge density effects, for ^1H NMR 89, 91
 - chemical equivalence 52
 - shift, *see also heteronuclei*
 - - aluminum-27 470
 - - boron-11 435
 - - ^{13}C , *see also carbon-13 NMR* 407 ff., 659 ff.
 - - difference, notation of 45
 - - fluorine-19 450 ff.
 - - ^1H , *see also proton chemical shift* 16, 29 ff.
 - - lithium-6, 7 464
 - - measurement 32 ff.
 - - nitrogen-15 439
 - - origin of 30
 - - oxygen-17 446
 - - phosphorus-31 459 ff.
 - - silicon-29 455 ff.
 - - tin-119 472 ff.
 - - transition metals, *see also heteronuclei* 474 ff.
 - - xenon-129 621
 - chemical exchange, *see dynamic NMR*
 - chemically induced nuclear polarization (CIDNP), *see also CIDNP* 604 ff.
 - chiral, liquid crystals 568
 - - enantiomeric excess 568, 569
 - shift reagents 219
 - chirality 211 ff.
 - and ^{13}C 224
 - influence on spectrum 216
 - 2-chloroacrylic acid, 2D INADEQUATE 333
 - COSY-DQF 308
 - chloroform 76
 - $^{13}\text{C}^1\text{H}$ coupling 76
 - chloroform-benzene complex 118
 - chromium acetylacetonate 243
 - CIDNP (chemically induced nuclear polarization) 604 ff.
 - AB system, spin polarized 609
 - dibenzoyl peroxide, thermal decomposition 605
 - energy polarization 605
 - entropy polarization 608
 - Kaptein rules 611
 - multiplet effect 608
 - Net effect 605
 - radical pair mechanism 606 ff.
 - radical pair, spin state 606
 - recombination product 607
 - transfer product 607
 - - AX system 610
 - spin polarized AB system 609
 - Wittig ether rearrangement 612
 - classical model, for NMR 16
 - clinical studies 640
 - CNDO method 85
 - coalescence point, *see also dynamic NMR* 505
 - coaxial tube 69
 - cobalt-59, *see also heteronuclei* 482 ff.
 - coherence 309
 - diagram 323
 - - COSY-90 324
 - double quantum 313, 326
 - level 322
 - order 328
 - transfer echo 325
 - COLOC 394
 - commutable operators 665

- complex spin systems 170
 - composite pulses 264
 - Computer, acquisition time 257
 - ADC, analog-digital-converter 254
 - bit, binary digit 255
 - digital analog converter (DAC) 256, 257
 - dwell time 257
 - dynamic range 256
 - memory locations 254
 - Nyquist theorem 257
 - resolution, of ADC 256
 - sampling rate 256
 - storage 254
 - word length 254
 - concentration dependence, of spectrum 72
 - constant time experiment 329
 - constraints 630
 - contact ion pairs (CIP) 586
 - contact shifts 597
 - continuous wave method (CW) 20 ff.
 - contour plot 284
 - copper-63, *see also* heteronuclei 484
 - coupling constants $^1\text{H}, ^1\text{H}$ 654 ff.
 - cyclopropanes 654
 - olefins 654
 - substituted benzenes 655
 - correlation time 240
 - COSY-90 experiment 296 ff.
 - AX system 61
 - experimental aspects 300 ff.
 - gradient enhanced 327
 - pulse sequence 61
 - COSY, *see* COSY-90
 - COSY-45 experiment 304
 - 2,3-bromopropionic acid 305
 - relative sign of coupling constants 305
 - COSY-DQF experiment 307
 - gradient enhanced 307
 - product operator treatment 320
 - COSY-LR (COSY long range) 305
 - coupling constant 43
 - reduced 43
 - sign 43
 - coupling mechanism 42
 - coupling, dipolar 22
 - Cr(acac)₃ 243
 - CRAMPS (combined rotation and multi-pulse NMR spectroscopy) 576
 - cross coils 19
 - cross peaks 296
 - cross polarization 365, 571
 - cryomagnet 24, 79, 638
 - cryoprobe 81, 82
 - ^{13}C satellites 76
 - CW method, *see* continuous wave method
 - cyclobutanes, substituted 213
 - cyclo-octatetraene dimer 225
 - cyclopropane, diamagnetic anisotropy 113
 - ring current 113
 - substituted 213
 - CYCLOPS phase cycle 266
 - cyclosilane [D₁₈] 83
- d**
- DANTE sequence 263
 - data flow 283
 - data improvement 269 ff.
 - decoupled COSY, ω_1 - 329
 - decoupling, broadband 275
 - GARP 277
 - gated- 382
 - heteronuclear 59, 273
 - homonuclear 58
 - in FT NMR 273
 - MLEV 277
 - noise- 275
 - off-resonance- 277
 - pulse methods 277
 - spin-spin 58
 - WALTZ-16 277
 - degeneracy 14
 - degenerate spin systems 226
 - bis*-dehydrobenzo[18]annulene, 2D NMR 298
 - delay time 259
 - delta scale 33 ff.
 - of carbon-13 407, 408
 - of heteronuclei 437
 - of protons in organic compounds 37
 - delta sigma ($\Delta\sigma$) 34
 - density matrix theory 309
 - deshielding 32
 - detection time t_2 61, 281
 - detector 19
 - phase-sensitive 259
 - deuterated solvents 68
 - deuterium-induced isotope shifts 593 ff.
 - deuterium quadrupole splitting 568
 - deuteriochloroform 67
 - diagonal peak 7, 60, 296
 - diamagnetic anisotropy 95
 - benzene 103
 - carbonyl group 98
 - cyclohexane 72
 - cyclopropane 113
 - nitro group 98
 - single bond 96
 - triple bond 97
 - diamagnetic effect 31

- shift 32
- susceptibility 94
- – exaltation of 110
- diastereomers 217, 294
- diastereomeric complexes 217
- diastereotopic molecules 220
- diatropic 104
- diatropicity, measurement 110
- dibromo-1,6-methano[10]annulene, 2,7- 222
- dichloroethene, *trans*-1,2- 226, 228
- diclorobenzene, 1,2- 76
- diffusion and field gradients 613
 - coefficient, measurement 612
- diffusion-controlled NMR 612 ff.
- diffusion-ordered spectroscopy (DOSY) 615
- difluoroethylene, spectrum 55
- difluoromethane, spectrum 55
- dihydroheptalene 225
- dimethyl-2-silapentane-5-sulfonate, [D₄]2,2- 70
- dinitrophenol, 2,4- 47
- dipolar coupling 22, 143, 241, 561
 - residual 565
 - – for AX system 566
 - – measurement by HMQC, HSQC 566
 - – ¹³C NMR spectrum of strychnine 567
- dipolar relaxation 241
- dipole-dipole relaxation 241
- disila[6]radialene 215
- distance ratio 355
- di-*n*-butylmercury, ¹⁹⁹Hg NMR 51
- 2D-NMR, *see two-dimensional NMR*
- 3D NMR 371ff.
- DNMR, *see dynamic NMR*
- DNP, *see dynamic nuclear polarization*
- DOSY (diffusion-ordered spectroscopy) 656
 - spectrum 616
- double bond shift, *n*-butyl-cyclo-octatetraene 540
- double quantum coherence (DQ) 307, 310, 313, 326
 - phenomena 307
 - selection, AX system 331
- double resonance, *see also decoupling* 58, 272 ff.
 - Bloch-Siegert shift 272
 - Hamilton operator 272
 - heteronuclear 59, 273
 - homonuclear 58, 272
- downfield 32
- DQ, *see double quantum coherence*
- DSS reference compound 70
- dwelt time 257
- dynamic NMR (DNMR):**
 - AB system, chemical exchange 519, 520
 - acetylacetone 549, 550
 - activation enthalpy 507
 - activation entropy 507
 - allylmagnesium bromide 542
 - [18]annulene 514, 531
 - annulenes, ring inversion 531 ff
 - – bond shift 531 ff.
 - approximate solution of DNMR analysis 509
 - – sources of error 509
 - Arrhenius activation energy 507
 - Arrhenius equation 507
 - Arrhenius plot 507
 - A-value 528
 - average life-times 505
 - averaging of parameters 505
 - benzene oxide, valence tautomerism 537
 - Bloch equations 505, 668
 - bond shifts 538 ff.
 - broadening due to inhomogeneity 509
 - bromocyclohexane, ring inversion 528
 - bullvalene, valence tautomerism 535
 - carbocations 545
 - carbon-13 and DNMR 512
 - chlorocyclohexane, ring inversion 528
 - coalescence point 505
 - complex exchange phenomena 512
 - COPE rearrangement 536
 - correlation times 504
 - cycloalkanes, ring inversion 522, 529
 - cyclohepta-1.3.5-triene, ring inversion 529
 - cyclohexane, ring inversion 526
 - cyclohexene, ring inversion 529
 - cyclo-octatetraene, double bond shift 538
 - – ring inversion 540
 - dicarbomethoxycycloheptatriene, valence tautomerism 537
 - dimethylcadmium 551
 - dimethylformamide *N,N*- 4, 501, 511
 - double bond shift 532
 - energy barrier 501, 506
 - enthalpy of reaction 508
 - entropy of reaction 508
 - equilibrium constant *K* 508
 - exchange broadening 509
 - exchange, of Larmor frequencies 501
 - – of AB ⇌ A₂ 519, 520
 - – approximate solution at coalescence 520
 - – complex phenomena 512

- dynamic NMR (DNMR):** (*contd.*)
- intermolecular 549
 - EXSY spectroscopy 515
 - spectrum of
 - 2,3-dimethylantraquinone-9-cyanimine 512, 516 ff.
 - ^{11}B , ^{11}B EXSY spectrum of halogen
 - exchange in boron halides 516, 519
 - carbon-13 EXSY spectra 516
 - phase of diagonal and cross peaks 515, 671
 - pulse sequence 516
 - rate constants, first order 505
 - by integration 516
 - pseudo first-order 552
 - Eyring equation 508
 - fast exchange 505, 509
 - fast relaxing nuclei, line broadening by 554
 - fluxional molecules 533
 - field strength influence 510
 - first order rate constants by integration 516, 520
 - first-order reactions 506
 - free energy of activation 508
 - frequency factor 507
 - hexamethylbenzene 545
 - hindrance to internal rotation 518
 - activation energies 519
 - 3,4-homotropilidene, valence tautomerism 533
 - intermolecular exchange 549
 - internal dynamics of organic molecules 517 ff.
 - internal rotation 501, 518 ff.
 - inversion of configuration 523 ff.
 - ammonia 523
 - diazines 524
 - diaziridine 524
 - trialkyloxonium salt 526
 - inversion recovery experiment 513
 - isomers of different energy 502
 - life-time τ 503
 - line broadening by fast relaxing neighboring nuclei 554
 - line shape, two-sites exchange 506
 - calculation 505
 - essential parameters 505
 - sources of error 509
 - metal carbonyl complexes 543
 - methanol 503
 - 2-methyloxepine 502
 - natural line width 509
 - norbornyl cation 546
 - organometallic compounds 542 ff.
 - oxepine, valence tautomerism 537
 - [6]paracyclophane, ring inversion 529
 - π -bond shift 538
 - population 505
 - pseudo rotation 526
 - rate constants, magnitude of 506
 - reaction enthalpy 508
 - reaction entropy 508
 - reaction kinetics 505
 - reaction order 506
 - ring inversion 526 ff.
 - annulenes 531
 - bromocyclohexane 528
 - chlorocyclohexane 528
 - cycloalkanes 522, 529
 - cyclohepta-1.3.5-triene 529
 - cyclohexane 526
 - cyclhexene 529
 - cyclo-octatetraene 538 ff.
 - [6]paracyclophane 529
 - slow exchange 505, 509
 - spin echo experiment 508
 - spin-spin splitting, loss of 503
 - substituted ethanes 521
 - temperature dependence of parameters 511
 - theoretical line shape 506
 - thiopene dioxide, influence of B_0 510
 - transition state theory 507
 - transmission coefficient 507
 - trimethylaluminium 550
 - two-dimensional exchange spectroscopy, *see* EXSY
 - valence tautomerism 532 ff.
 - benzene oxide 537
 - bullvalene 535
 - cyclo-octatetraene 538 ff.
 - dicarbomethoxycycloheptatriene, 537
 - 3,4-homotropilidene 533
 - oxepine 537
 - van't Hoff equation 508
- dynamic processes, in the solid 588 ff.
- dynamic nuclear polarization (DNP) 623 ff.
- cross effect (CE) 623
 - dissolution DNP (D-DNP) 623
 - Overhauser DNP (O-DNP) 623
 - in liquids 624
 - polarizing agents 624
- solid state DNP (SS-DNP) 623
- dynamic range 256, 269

e

echo-planar imaging (EPI) 337
 echo signal 249
 E.COSY (exclusive correlation spectroscopy) 628
 eddy currents 615
 editing 383
 effective Larmor frequencies 226, 628
 eigenfunction 14, 152
 eigenstate 14, 151
 eigenvalue problem 173
 eigenvectors 171
 electric field effect 114
 – in nitrobenzene 115
 – in pyridine 115
 – linear 115
 – quadratic 116
 electromagnetic spectrum 23
 electron density, on neighboring carbon 87
 electronegativity 87, 451
 electron on a circle 105, 152
 electron paramagnetic resonance (EPR) 623
 – spin resonance (ESR) 623
 electron-nuclear double resonance (ENDOR) 623
 empirical substituent constants, for protons 121, 652 ff.
 – for carbon-13 418 ff., 662
 enantiomeric excess 568, 569
 enantiomers 217
 enantiotopic molecules 220
 ENDOR (electron-nuclear double resonance) 623
 energy difference 15, 19
 energy, of spin states 14
 – level diagram 44
 – – A_2 system 161
 – – AA'XX' system 196
 – – AB system, $J = 0$ 157
 – – AB_2 system 180
 – – ABX system 184
 – – AX system 44
 – separation 15
 enhancement factor, NOE 344
 enhancement factors, table of 361
 enzyme spectrum 629
 EPR (electron paramagnetic resonance) 623
 Ernst angle 258
 ESR (electron spin resonance) 623
 estrone, spectrum 80
 ethylbenzene 78, 255
 ethyl formate 35, 41
 ethynylphenantrene, proton deshielding 97
 europium, shift reagents 603 ff.

Eu(FOD)₃-induced contact shifts 604
 evolution time t_1 61, 281
 exaltation, of diamagnetic susceptibility 110
 exchange, *see also dynamic NMR* 501
 – broadening, *see also dynamic NMR* 509
 excitation 21
 – selective 260 ff.
 exponential multiplication 269 ff.
 external standard 70
 – correction for 71
 extreme narrowing limit 241
 EXSY spectroscopy 514 ff.
 Eyring equation 508
 E,Z-isomers 294

f

Fermi contact mechanism 42
 FID, *see free induction decay*
 field effect, *see electric field effect*
 field gradients 75, 326, 612, 644
 – homogeneity 75
 – strength 79
 field sweep 21
 field/frequency ratio 33, 75
 filter functions 285
 first order approximation 167, 181
 first-order rules 45, 46
 – spectra 45
 flemingin B 215
 flip angle 239
 flip-flop mechanism 244
 – heteronuclear 366
 – homonuclear in solids 365
 fluorenyllithium, TMEDA complex, solid state NMR 588
 fluorine-19 447 ff.
 fluorine shielding 32, 450
 fluoropyridine, 2-, *J*-resolved spectrum 295
 fluxional molecules 533
 folding 264, 267
 formaldoxim 72
Fourier transform spectroscopy 13, 21, 233 ff.
 – acquisition time 257
 – complications 267 ff.
 – composite pulses 264
 – computer, *see above*
 – data collection 257, 273
 – data improvement 269 ff.
 – decoupling 273
 – delay time 259
 – digitizer 256
 – dwell time 257
 – double resonance 273

Fourier transform spectroscopy (*contd.*)

- dynamic range 269
- filter functions 272
- frequency folding 264, 267
- intensity measurements 269
- presaturation 269
- parameters 257
- phase cycles 266
- phase error 259 ff.
- presaturation 269
- pulse calibration 263, *see also pulse and pulses*
- quad-images 265
- quadrature detection 265
- repetition time 250, 262
- sampling rate 256
- single detection 264
- spectral width 257, 267
- time domain 253
- time sequence 259
- weighting functions 272
- window functions 272
- word length 254
- zero-filling 272
- Fourier transformation 283
- free induction decay (FID) 21, 22, 61, 76, 238, 253
 - measurement 79
- frequency-dependend phase error 259
- frequency, domain 252
 - filter 264, 268
 - folding 264, 267
 - sweep 21
 - precision 77
- frog muscle 643
- FT NMR, *see* Fourier transform spectroscopy
- FT NMR spectrometer 254 ff.
 - diagram 256
- fullerenes 416
- furan, ¹H spectrum 55
- F_z operator 665

g

- γ-effect 419
- GARP 277
- gated decoupling 382
- GAUSS pulse, excitation profile 262
- GAUSSIAN method 85
- geminal, ¹H, ¹H coupling 123
 - and hybridization 123
 - effect of substituents 124 ff.
 - MO model 126
 - neighboring π-bonds 124
 - ¹³C, ¹H coupling 425

- geminate pair 608
- g-factor 608
- glucose α-D- and β-D-, 1D TOCSY spectrum 370
- glycolysis 642
- gradient enhanced NMR 326 ff.
- gyroscope 234

h

- Haasnoot-Altona equation 638
- hairpin 632
- half-width, of signal 247
- Hamilton matrix 173
- Hamilton operator 151, 153, 314
 - for isotropic mixing 367
 - for partially oriented systems 560
 - for solid state NMR 570
 - for spin-decoupling 272
 - in polar coordinates 664
- hard pulses 260
- Hartmann-Hahn experiment, *see also* HOHAHA, HEHAHA 364 ff.
 - in liquids 366 ff.
 - in solids, pulse sequence 367
- H, D coupling 229
 - substitution 228
- HEHAHA (heteronuclear Hartmann-Hahn) experiment 366
- Henderson-Hasselbalch equation 94
- Herzfeld-Berger method 573
- heteronuclear two-dimensional shift correlations** 389 ff.
 - HETCOR experiment 389
 - pulse sequence 391
 - spectrum of a paracyclophane 399
 - of 2,7-dilithionaphthalene 393
 - of angelica acid 398
 - of *bis*-dehydrobenzo[20]annulene 399
 - of tiglic acid 398
 - HETCOR COLOC 394
 - HMBC experiment 394
 - gradient enhanced 397
 - spectrum of 3-fluorophenanthrene 397
 - HMQC experiment 391
 - ¹³C, ²H shift correlation with BIRD pulse 396
 - pulse sequence 391
 - spectrum of
 - benzo[c]1,7-methano[12]annulene 393
 - with single quantum A elimination by BIRD 394
 - HSQC experiment 391
 - pulse sequence 391
- heteronuclei** 431 ff.

- **aluminum-27** 468 ff.
 - chemical shifts 469,470
 - multiple quantum MAS (MQMAS) 469
 - referencing 469
 - spin-spin coupling 471
 - asymmetry parameter 433, 587
- **boron-11** 435 ff.
 - chemical shifts 438
 - COSY spectrum 440
 - polyhedral boranes 438
 - referencing 437
 - selected compounds 439
 - spin-spin coupling 438
- chemical shift anisotropy 434
- chemical shifts 433, 437
- classification 432
- **cadmium-113** 488 ff.
 - chemical shifts 488
 - referencing 488
 - spin-spin coupling 489
- **cobalt-59** 482 ff.
 - chemical shift 483, 484
 - referencing 483
 - spin-spin coupling 483
- **copper-63** 484
 - chemical shifts 484
- CSA mechanism, for relaxation 434
- **fluorine-19** 447 ff.
 - chemical shifts 448 ff.
 - of methylhalides 448 ff.
 - of selected fluorides 448 ff.
 - of selected organic fluorine compounds 451
 - referencing 448
 - spectra 450
 - spin-spin coupling 452
 - in organic fluorine compounds 453
 - through-space coupling 454
- INADEQUATE, 1D ^6Li , ^6Li 468
- intensity enhancements 485
- **iron-57** 489 ff.
 - chemical shifts 491
- **lithium-6,7** 462 ff.
 - 1D ^6Li , ^6Li INADEQUATE 468
 - 1D HMQC 466
 - 2D HMQC 466
 - aggregates 465
 - chemical shifts 463, 464
 - ring current effect 464
 - referencing 463
 - solid state NMR 467, 586
 - spin-spin coupling 464 ff.
 - multiplets 464 ff.
- magnetic strength, of hetero nuclei 432
 - main group metals 462 ff.
- **manganese-55** 491 ff.
 - chemical shifts 491
 - spin-spin coupling 492
- **mercury-199** 494 ff.
 - chemical shifts 495
 - referencing 495
 - relaxation 494
 - satellite spectra 494
 - spin-spin coupling 495
- **molybdenum-95** 492
 - natural abundance 432
- **nitrogen-15** 439 ff.
 - adenosine, interaction with metal salts 444
 - chemical shifts 442
 - metal salt interaction 444
 - INEPT 440
 - spectrum of pteridine 441
 - inverse detection 440
 - NOE 440
 - protonation shifts 443
 - 7-methylpurine, spectrum 444
 - referencing 443
 - spin-spin-coupling 445
 - nuclear properties 436, 437, 475, 478
- **osmium-187** 496
- **oxygen-17** 445 ff.
 - acoustic ringing 446
 - chemical shifts 446
 - measurement 445
 - referencing 446
 - RIDE sequence 446
 - spin-spin-coupling 447
- **phosphorus-31** 458 ff.
 - chemical shifts 459
 - coordination number 458, 459, 461
 - dependence on P-P-P bond angle 462
 - effect of charge 460
 - of phosphines important for homogeneous catalysis 460
 - ranges for different bonding situations 460
 - diphosphanes, conformation 460
 - referencing 458
 - spin-spin coupling 461
- **platinum-195** 480 ff.
 - chemical shifts 480
 - relaxation 480
 - spin-spin coupling 481, 482
- quadrupolar nuclei 432
 - coupling constant 433
 - electric field gradient 433
 - line width 433

heteronuclei (*contd.*)

- relaxation times 433
 - quadrupole moment 433
 - reference compounds 434
 - reference, universal 434
 - **rhodium-103** 485 ff.
 - chemical shifts 486
 - spin-spin coupling 487
 - Tolman angle 487
 - RIDE (ring down elimination) sequence 446
 - RIDE spectrum 447
 - sagging behavior 454, 458
 - semimetals 435 ff.
 - **silicon-29** 454 ff.
 - chemical shifts 454 ff.
 - methylsilanes 455
 - sagging behavior 454, 458
 - NOE 454
 - referencing 454
 - satellites, ^{29}Si , ^{13}C , in ^{29}Si spectrum 457
 - spin-spin coupling 457
 - ranges of Si, X coupling 458
 - satellite lines 457
 - **tin-119** 471 ff.
 - chemical shifts 472, 473
 - inverse detection 471
 - magnetically active isotopes 471
 - referencing 472
 - satellites in ^1H spectra 471
 - spin-spin coupling 473
 - transition metals 474 ff.
 - nuclear properties 475
 - referencing 478 ff.
 - chemical shift ranges 478 ff.
 - \mathcal{E} -values 478 ff.
 - Tolman angle 487
 - **tungsten-183** 492 ff.
 - chemical shift 493
 - COSY spectrum, ^{183}W , ^{183}W 493
 - spin-spin coupling 493
 - universal reference \mathcal{E} 434
 - **vanadium-51** 476 ff.
 - chemical shifts 477, 480
 - spin-spin coupling 480
 - **xenon-129** 621 ff.
- heterolock 75
- heterotactic 223
- high resolution NMR 153
- higher order spectra 56
- high-field magnet 24, 79, 638
- high-resolution solid state NMR** 568 ff.
- assignment methods 576
 - NQS (non quaternary carbon suppression) 576
 - J -resolved spectroscopy 577
 - spectrum of camphor 577
 - side band suppression by TOSS 573
 - by SELTICS 573, 575
 - alkalide 584, 585
 - anisotropy of chemical shift 571
 - adsorbed molecules 583
 - applications, spin $\frac{1}{2}$ nuclei 580 ff.
 - ^{13}C CP/MAS spectra of aromatics adsorbed on Al_2O_3 585
 - ^{13}C CP/MAS NMR spectrum of 2-methylal zinc chloride 581
 - ^{13}C CP/MAS spectra of aromatics adsorbed on Al_2O_3 585
 - ^{29}Si CP/MAS NMR spectrum silica-60 582
 - ^{29}Si , ^{29}Si 2D INADEQUATE spectrum of the zeolite ZMS-12 584
 - ^{29}Si MAS NMR spectrum of aluminosilicate analcite
 - silicates, chemical shift range 583
 - ^{119}Sn CP/MAS NMR spectrum tetramethylactelyd tin 581
 - asymmetry parameter 586, 587
 - caesium NMR
 - caesium-133 spectrum 586
 - chemical shift tensor 571
 - anisotropy, angular term 572
 - contact ion pairs (CIP) 586
 - cross polarization (CP) 571
 - dipolar coupling, intermolecular 569
 - double rotation (DOR) 579
 - dynamic processes, in the solid 588 ff.
 - ^{13}C MAS spectrum of fluorenyllithium(TMEDA) 588
 - EXSY spectroscopy 589
 - $T_{1\rho}$ measurements 589
 - electrone 585
 - experimental techniques 570
 - Hamilton operator 570
 - Hartmann-Hahn experiment 571
 - high power ^1H decoupling 569
 - high-resolution CP/MAS spectrum 573
 - line narrowing 569, 570 ff.
 - for adsorbed molecules, ^{13}C , ^1H NMR 585
 - lithium NMR 584 ff.
 - lithium-7 585
 - magic angle spinning (MAS) 567, 569
 - magic angle 572
 - multiple quantum MAS 579

- powder spectra, molecules with axial symmetry 572
- - molecules without axial symmetry 572
- quadrupolar nuclei 572, 577 ff.
- - energy level diagrams for $I = 1$ and $I = 3/2$ 578
- quadrupole coupling constant 578, 585 ff.
- rotational side bands 574
- rotor 572
- sample rotation 573, 574
- side band suppression by TOSS 573
- - by SELTICS 573
- - - pulse sequence 575
- - - spectrum of tyrosine hydrochloride 575
- solvent-separated ion pairs (SSIP) 586
- spectrum of solid triphenylmethyl lithium quinuclidine 587
- spin-flip narrowing 574
- spinning rate 572
- - effect for ^{31}P NMR of triphenylphosphine 574
- static ^2H solid state NMR spectra 579
- WAHUA-sequence 575, 576
- zeolite 584
- hindered rotation 518 ff.
- HOESY (heteronuclear NOE) 355
- pulse sequence 355
- spectrum 356
- HOHAHA (homonuclear Hartmann-Hahn) experiment 366
- homoallyl $^1\text{H}, ^1\text{H}$ coupling 141
- 3,4-homotropilidene, valence tautomerism 533 ff.
- EXSY spectrum 534
- Hückel MO calculation 107
- Hückel rule 104
- Huggins electronegativity 638
- human skull 646
- hump test 77
- hydrogen bonding 117
- fluoride 42
- hyperpolarization 617 ff.
- i*
- IGLO method 85
- imaging, by NMR 642
- impurities, paramagnetic 73
- INADEQUATE experiment, 1D, $^{13}\text{C}, ^{13}\text{C}$ 400
- INADEQUATE experiment 2D, $^1\text{H}, ^1\text{H}$ 331
- o-disubstituted benzenes 334
- p-disubstituted benzenes 334
- adenosine 336
- product operator formalism 332
- INADEQUATE experiment, 2D $^{13}\text{C}, ^{13}\text{C}$ 402
- indirect or scalar coupling, *see also* spin-spin coupling 43
- INDO method 85
- INEPT, pulse sequence 360 ff.
- enhancement factor 360
- indirect 363
- inverse 363
- multiplicities 361
- of NH group 362
- product operator formalism 363
- refocused 361
- reverse 363
- signal-to-noise ratio 364
- INEPT⁺ 361
- inorganic phosphate 642
- integration 35 ff., 77
- intensity distribution, for AX_n systems with $I(X) = 1, 3/2$ 664
- intensity, relative 47
- interferogram 253
- intermolecular exchange, *see also* dynamic NMR 549
- internal rotation, *see also* dynamic NMR 518 ff.
- internal standard 70
- intersystem crossing 607
- intramolecular NOE 348
- intrinsic isotope effect 592
- inverse probe head 81
- inverse INEPT 363
- signal-to-noise ratio 364
- inversion of configuration, *see also* dynamic NMR 523 ff.
- inversion recovery experiment 247, 248, 640
- for ^{13}C , *m*-xylene 381
- for rate constant determination 513
- in-vivo* NMR 640
- irreducible representation 181
- isochronous nuclei 52
- isodynamic 533
- isomerism 211 ff.
- isotactic polymers 223
- isotope effects, in NMR 591
- $\Delta^{13}\text{C}(^2/^1\text{H})$, cyclohexane 593
- $\Delta^{15}\text{N}(^{18}/^{16}\text{O})$, sodium nitrate 593
- empirical correlation 592, 594
- intrinsic isotope effect 592
- isotopic perturbation of equilibrium 597 ff.
- ^{18}O isotope shifts for carbonyl groups 595
- potential curve for vibrational states 593
- primary isotope effect 591
- secondary isotope effect 591

- isotope effects, in NMR (*contd.*)
 - SNIF (site specific natural isotope fractionation) 595
 - isotopic perturbation of equilibrium 595
 - isotropic coupling 367
 - isotropic mixing 366
 - iterative analysis 206 ff.
- j**
- Jeener experiment 296
 - modification of 304
 - J* coupling, *see* spin-spin coupling
 - J*, δ spectra, *see* *J*-resolved spectra
 - Joule-Thomson effect 81
 - J*-resolved spectra 289 ff.
 - applications 291
 - *n*-butylbromide 293
 - data treatment 293
 - EXCORCYCLE 295
 - fluoropyridine 295
 - ghost signals 295
 - heteronuclear 373
 - – pulse sequence 373
 - homonuclear 291
 - measuring time 295
 - of mixture 293
 - phantom signals 295
 - practical aspects 294 ff.
 - jump-and-return 640
- k**
- Kaptein rules 611
 - Karplus curve, $^3J(^1\text{H}, ^1\text{H})$ 129, 631, 638
 - $^{13}\text{C}, ^{13}\text{C}$ 423
 - $^{13}\text{C}, ^1\text{H}$ 427
 - Haasnoot-Altona 638
 - in peptides 631
 - in oligo- and polysaccharides 638
 - $^{31}\text{P}, ^1\text{H}$ 636
 - keto-enol equilibrium 549
 - ketones, protonated 67
 - unsaturated 99
- l**
- laboratory frame 234
 - lactate formation 642
 - Lamb formula 31, 409
 - Landé- or g-factor 606
 - lanthanide complex 601 ff.
 - induced shift (LIS) 601 ff.
 - Laplace operator 152
 - LAOCOON program 207
 - Larmor frequency 16, 21
 - Larmor precession 234
 - LCAO (linear combination of atomic orbitals) 481
 - leakage factor 624
 - LEFE (linear electric field effect) 115
 - life sciences 641
 - life-time 503
 - line broadening 22, 73, 494
 - by fast relaxing neighboring nuclei 554
 - narrowing 570
 - shape 246, 285
 - splitting 43
 - width 76, 246
 - linear combination 160
 - linear electric field effect 115
 - linearly polarized field 237
 - liquid crystals 82
 - NMR in 558
 - liquids, NMR in 22
 - LIS (lanthanide induced shift) values 601
 - lithium-6, 7, *see also* heteronuclei 462 ff.
 - living objects 641
 - local diamagnetic contribution to the shielding constant 86
 - local field 30
 - lock level 76
 - signal 75
 - long-range correlation, 2D, $^{13}\text{C}, ^1\text{H}$ 394
 - $^1\text{H}, ^1\text{H}$ (COSY-LR) 305 ff.
 - long-range coupling, $^1\text{H}, ^1\text{H}$ 137 ff.
 - M (W) mechanism 138
 - saturated systems 138
 - unsaturated systems 139
 - longitudinal or spin-lattice relaxation 237
 - relaxation time 237, 239
 - Lorentz curve 253
 - Lorentz-Gauss transformation 270
 - Lorentzian line shape 246
 - lowering operator 154, 312
 - low-pass filter 330
 - L-valin 219
- m**
- macroscopic sample, pulse excitation 236 ff.
 - magic angle 23
 - spinning 433, 569, 625
 - magnet, superconducting, *see also* cryomagnet 24, 79, 638
 - magnetic anisotropy, *see* diamagnetic anisotropy
 - magnetic dipole 14
 - equivalence 52 ff.
 - field, local 16
 - – increase of field strength 79
 - moment 13, 14, 16
 - non-equivalence 220

- properties of nuclei 25, 432, 436, 475
 - quantum number 14
 - resonance imaging (MRI) 642 ff.
 - magnetization 70
 - macroscopic 21
 - magnetogyric ratio 13
 - magnitude or absolute value representation 285
 - main group metals 464
 - manganese-55, *see also* heteronuclei 492
 - McConnell equation 95
 - medicine, NMR in 626 ff.
 - mercury-199 495
 - memory locations 254
 - metabolic changes 642
 - metal carbonyl π -complexes, $\delta(^1\text{H})$ 120
 - metal hydrides, proton resonances in 120
 - 1,6-methano[10]annulene, spectrum 107, 109
 - 1,6-methano[10]annulene, dianion, $\delta(^1\text{H})$ 107
 - 1,7-methano[12]annulene, spectrum 109
 - methoxygalactose 96
 - microcell 676
 - mixing operator 366
 - time 366
 - mixture of *n*-butyl halides 299
 - MLEV pulse method 277
 - molecular, biology 625 ff.
 - motion 241
 - symmetry 211 ff.
 - MO model for $^2J(^1\text{H}, ^1\text{H})$ 126
 - molybdenum-95, *see also* heteronuclei 494
 - MRI (magnetic resonance imaging) 642 ff.
 - multidimensional experiments 80, 371, 373
 - 3D NMR principle 373
 - NOESY-TOCSY sequence 375
 - multiple quantum, coherence 312
 - MAS solid state experiment 469, 579
 - multinuclear probe head 81
 - multiplicity, of NMR signals 41, 46, 201
 - selection by SEFT, APT 383
 - – by DEPT (distortionless by polarization transfer) 387
- n**
- NAD⁺, ¹H nmr spectra at different B_0 fields 626
 - 2D ¹³C, ¹³C INADEQUATE experiment 402
 - naphthalene, ring current 103
 - naphthobiphenylene, COSY-LR 307
 - natural abundance 26, 50
 - natural products 625
 - neighboring group 32
 - π -bonds 124
 - nematic phases, *see also* liquid crystals 558
 - nicotinamide adeninedinucleotide (NAD⁺) 402, 626
 - NICS values (nucleus independent chemical shift) 111, 416
 - ortho*-nitroanilin, COSY spectrum 297
 - COSY-LR 306
 - nitrobenzene, electric field effect in 115
 - nitrogen-15, *see also* heteronuclei 441 ff.
 - nitropropane, ¹H NMR spectrum of 89
 - NMR, frequency increase for ¹H 79
 - other nuclei, tables 26, 436, 475
 - signal 20
 - spectrometer, *see* below
 - thermometer for measurements at variable temperature 82
 - NOE difference spectroscopy 346 ff.
 - assignment of ¹H configuration 347
 - NOE (nuclear Overhauser effect) 343 ff.
 - NOESY, Bloch vector diagram 351
 - spectrum, of [6]paracyclophane-8,9-dimethylbicarboxylate 354
 - – of benzo[*b*]biphenyldication, 352
 - distance ratio 355
 - product operator formalism 353
 - pulse sequence 351
 - NOESY-TOCSY, 3D pulse sequence 375
 - noise decoupling 275
 - non-alternating hydrocarbons 104
 - nonbonding electron pairs 124
 - nonplanar annulene 109
 - normalized function 155
 - NQR (nuclear quadrupole resonance) 26
 - N-type signal 325
 - nuclear Overhauser effect 80, 341 ff.
 - ¹³C{¹H} 345
 - complications 348
 - dependence on $\omega_0\tau_c$ 350
 - distance measurements 345
 - enhancement factors 81, 344, 361, 485
 - – table 361, 485
 - heteronuclear 345
 - heteronuclear, 2D (HOESY) 355 ff.
 - homonuclear, 1D 345
 - homonuclear 2D (NOESY) 350 ff.
 - – Bloch vector diagram and pulse sequence 351 ff.
 - signal enhancement 344
 - spin diffusion 349
 - nuclear properties, tables 26, 436, 475

- nuclear quadrupole moment 25
 - quadrupole resonance (NQR) 26
 - spin operators 154
 - spin vector 42
 - Zeeman splitting 15
- nuclei, even-even 25
 - even-odd 25
 - odd-odd 25
- nucleic acids, *see also bio-NMR, nucleic acids* 634 ff.
- Nyquist theorem 257
- o**
- off-diagonal matrix elements 171
- off-resonance decoupling 277
- oligosaccharides, *see also bio-NMR, oligo- and polysaccharides* 636 ff.
- one-dimensional homonuclear NOE 345 ff.
 - intramolecular 348
 - NOE difference spectroscopy 346
- one-dimensional INADEQUATE sequence 398 ff.
- one-dimensional selective TOCSY 368
- operators, evolution of 313 ff.
- optical isomers 217
 - pumping 621 ff.
 - purity, by NMR 217
- optically active center, intramolecular 219
- order matrix or order tensor 565
- order parameter 561
- organic molecules, proton resonances in 122 ff.
- organic molecules, spin–spin coupling constants in 144
- organometallic compounds, $\delta(^1\text{H})$ 119
 - dynamic processes 542
- orthogonal function 155
- ortho*-hydrogen 617
- ortho*-coupling 201
- osmium-187, *see also heteronuclei* 498
- O-DNP (Overhauser dynamic nuclear polarization) 623, 624
- Overhauser enhancement 81, 344
- Overhauser effect, original 341
- oxygen, line broadening effect 73
- oxygen -17, *see also heteronuclei* 447
- p**
- [6]paracyclophane-8,9-dimethylbicarboxylate, NOESY spectrum 354
- para*-hydrogen induced polarization (PHIP) 618
- para*-hydrogen 617 ff.
- paramagnetic, shift 32
 - materials 597 ff.
 - – contact shifts 597
 - – pseudo-contact shifts 599
 - – shift reagents 599
 - moment 31
 - ring current effect 105
 - paratropic molecules 106
 - partial orientation 558
 - partially oriented molecules, *see also alignment* 557 ff.
 - in chiral liquid crystals 568
 - in nematic phases of liquid crystals 558 ff.
 - – benzene, spectrum of partially oriented 562
 - – dipolar coupling 561
 - – order parameter 561
 - – oriented A_2 system 560
 - – Saupe matrix 563
 - – spectral analysis 563
 - – spectrum of partially oriented methylene chloride 559
 - – structural data for cyclopropane 564
 - – structure determination 563
 - – – for cyclobutane 564
 - – – for ethylene 564
 - residual dipolar couplings, *see also individual entry* 565
 - particle spin 181
 - PASADENA, AX system 618
 - Pascal's triangle 172
 - passive, coupling 628
 - spin 43, 183
 - PBLG (poly- γ -benzyl-glutamate) 567
 - pentachloropropane, 1,1,2,3,3-, spectrum 57
 - peptide partial structure, NMR experiments 630
 - peptides, *see also bio-NMR, peptides and proteins* 627 ff.
 - perfused organs 641, 643
 - perturbation of equilibrium 595
 - PFGSTE (pulsed field gradient stimulated echo experiment) 614, 615
 - PFT NMR, *see Fourier transform spectroscopy*
 - PGSE (pulsed field gradient spin echo) 613, 614
 - pH, and proton chemical shift 93
 - in the cell 642, 643
 - phase, behavior in 2D NMR 671
 - correction 261
 - – by spin echo experiment 287
 - cycles 266, 322 ff.
 - error 259, 260
 - modulation 282
 - shift 301

- phasesensitive 2D spectra 266
- phenylacetylene hydrogenation, PHIP spectrum 619
- PHIP (*para*-hydrogeninduced polarization) 618
- measurements 620
 - polarization transfer 620, 621
 - product operator formalism 620
 - spectra 619
- phosphorus-31 NMR, *see also heteronuclei* 641 ff.
- π -complexes, $\delta(^1\text{H})$ 120
- π -electron density, ^1H NMR 89
- ^{13}C NMR 410 ff.
- pK_a determination 93
- platinum-195, *see also heteronuclei* 482 ff.
- polarization transfer 357 ff.
- polyacetylenes, long-range ^1H , ^1H coupling 142
- polyhedral boranes 440
- polypeptides, ^{13}C , ^{15}N enriched, scalar coupling 633
- polymer spectroscopy 223
- poly- γ -benzyl-glutamate (PBLG) 567
- polysaccharides, *see also bio-NMR, oligo- and polysaccharides* 636 ff.
- preparation time 281
- presaturation 269, 640
- primary isotope effect 591
- probability, of transition 19
- probe 25
- probe head 25, 77
- cryo 81
 - inverse 81
 - multinuclear 81
- product operator formalism 309 ff.
- coherence 309
 - COSY experiment within 317
 - double quantum coherence 313
 - multiple-quantum coherences 312
 - observables 316
 - operator basis for AX system 311
 - operators, evolution of 313
 - single quantum coherence (SQ) 307, 310
 - zero-quantum coherences 310
- propionamide, ^1H spectrum 39
- propylnaphthalene, hyperfine coupling 599, 600
- proteins, *see also bio-NMR, peptides and proteins* 627 ff.
- proton chemical shift** 650 ff.
- aldehydes 99, 651
 - and electronegativity 87
 - and structure 85
 - annulenes 104 ff.
 - anthracene 103
 - aromatic ions 89, 90
 - aromatic protons 651
 - carbanions 92
 - carbocations 92
 - charge density at carbon 89
 - charge density effects 91
 - diamagnetic anisotropy 87, 95
 - diamagnetic susceptibility 94
 - dimethyl-15,16-dihydropyrene, *trans*-15,16-dianion, $\delta(^1\text{H})$ 107
 - electric field effect 114
 - electron density 87
 - ethyl halides 87
 - for selected organic compounds 38
 - hydrogen bonding 117
 - induced magnetic moments 94
 - inductive effect 89
 - McConnell equation 95
 - methano[10]annulene 1,6-, dianion, $\delta(^1\text{H})$ 107
 - methano[10]annulene, 1,6- 104
 - methano[12]annulene, 1,7- 108
 - methyl derivatives 88
 - methyl protons 650
 - methylene protons 650
 - naphthalene 103
 - neighboring atoms, influence of 86
 - NICS values 111
 - olefinic protons 651
 - origin of 86 ff.
 - π -electron density 89
 - pH dependence 93
 - ring current 101 ff.
 - - [18]annulene 104
 - - annulenes 104 ff.
 - - cyclopropane 113
 - - dimethyl-15,16-dihydropyrene, *trans*-15,16-dianion $\delta(^1\text{H})$ 107
 - - intensity 108
 - - methano[10]annulene 1,6-, dianion, $\delta(^1\text{H})$ 107
 - - methano[10]annulene, 1,6- 104, 107
 - - methano[12]annulene, 1,7- 108
 - - non-alternating hydrocarbons 104
 - - paramagnetic 106
 - - *trans*-15,16-dimethyl-15,16-dihydropyrene 104
 - - tricycloazines 109
 - Shoolery rule 652
 - solvent effects 120 ff.
 - substituent constants 121
 - substituent effect 652

- proton chemical shift (*contd.*)
 - for methanes 652
 - for substituted benzenes 653
 - van-der-Waals effect 86, 114, 116
 - proton coupling constants and chemical structure, *see also spin-spin coupling* 122 ff.
 - dipolar coupling 143
 - geminal coupling 122, 123 ff.
 - long-range coupling 122, 137 ff.
 - through-space coupling 143
 - vicinal coupling 122, 128 ff.
 - proton screening 86
 - shielding 32
 - pseudo contact shifts 599
 - P-type signal 325
 - pulse angle 77, 239
 - calibration 263
 - excitation 234
 - frequency 33
 - length 22
 - r.f. 21
 - sequence 296
 - width t_p 250, 258
 - pulsed field gradient, spin echo (PGSE) 613
 - stimulated echo (PFGSTE) 614, 614
 - pulses, selective 261
 - soft 261
 - BIRD 329
 - GAUSS 262
 - composite 263
 - hard 260
 - pyramidal atomic inversion 525
 - pyridine, electric field effect 115
 - pyrogallol (1,2,3-trihydroxybenzol) 178
 - Pythagoras 176, 236
- q**
- quad-images 265
 - quadratic field effect 116
 - quadrature detection 265
 - quadrupolar nuclei 568, 577, 584
 - relaxation 243, 433
 - coupling 433, 568, 586
 - moment 25
 - splitting for nuclei with $I = 1$, angular dependence 568
 - for deuterium 568
 - quadrupole relaxation 243, 433
 - quantization 14
 - quantum condition 13, 105, 153
 - mechanical formalism 151
 - number 14
 - theory 13
 - quantum mechanical model for isolated proton 13
 - angular momentum 13
 - eigenfunctions 14
 - magnetic dipole 14
 - magnetic quantum number 13
 - magnetogyric ratio 13
 - nuclear Zeeman splitting 15
 - quantized magnetic moment 13
 - quantum condition 13
 - spin quantum number 14
 - wave functions 14
- r**
- Rabi experiment 18
 - racemate 217
 - radiation, electromagnetic 16
 - radiofrequency (r.f.) 19
 - radicals 601
 - radiofrequency impulses 237
 - radiation 19
 - radiology 646
 - raising operator 154
 - rare nuclei 49
 - rate constants, determination of 515
 - ratio $J(\text{H,H})/J(\text{H,D})$ 229
 - $J/\nu_0\delta$, significance of 56
 - receiver 21
 - coil 16
 - gain 77
 - signal 252 ff.
 - receptivity 26
 - rectangular pulse, excitation profile 262
 - REDOR (rotational echo double resonance) 580
 - reduced coupling constant 43
 - reference compound 33, 67, 70, 434, 439
 - aluminum-27 471
 - fluorine-19 450
 - lithium-6,7, 465
 - nitrogen-15 443
 - oxygen-17 448
 - phosphorus-31 460
 - proton
 - silicon-29 456
 - tin-119 474
 - transition metals 478 ff.
 - relative intensity 47
 - relaxation 21, 23, 239 ff., 243
 - by chemical exchange 246
 - by chemical shift anisotropy 43
 - by paramagnetic species 242
 - by scalar coupling 243
 - in the rotating frame ($T_{1\rho}$) 247, 580, 587

- quadrupole - 243, 433
 - rate constant R_1 240
 - reagent $[\text{Cr}(\text{acac})_3]$ 243
 - spin rotation 243, 482
 - spin-lattice or longitudinal - 239
 - spin-spin or transverse - 23, 234, 243
 - time measurements 247 ff
 - - longitudinal (T_1) 237, 239
 - - - inversion recovery experiment 247
 - - transverse (T_2)
 - - - spin echo experiment 248 ff.
 - relayed spectra 367
 - repetition time t_r 250
 - residual dipolar couplings, *see also* dipolar coupling 565 ff.
 - resolution 76
 - of ADC 256
 - resonance condition 16
 - equation 17
 - frequency 16, 26, 436, 475
 - reverse INEPT 363
 - signal-to-noise ratio 364
 - RF (r.f.) pulse 21, 237
 - RF source 19, 258
 - rhodium-103 487, *see also* heteronuclei, 485 ff.
 - ring current 101 ff.
 - [18]annulene 104
 - annulenes 104 ff.
 - cyclopropane 113
 - dimethyl-15,16-dihydropyrene, *trans*-15,16-dianion $\delta(^1\text{H})$ 107
 - intensity 108
 - methano[10]annulene 1,6-, dianion, $\delta(^1\text{H})$ 107
 - methano[10]annulene, 1,6- 104, 107
 - methano[12]annulene, 1,7 108
 - non-alternating hydrocarbons 104
 - paramagnetic 106
 - *trans*-15,16-dimethyl-15,16-dihydropyrene 104
 - tricycloazines 109
 - ring inversion, *see also* dynamic NMR 526 ff.
 - ROESY effect, dependence on $\omega_0\tau_c$ 371
 - experiment 369
 - spectrum, trisaccharide 372
 - roof effect 56
 - rotating field vector 235
 - frame 235
 - - experiments 364 ff.
 - - - HEHAHA 366
 - - - HOHAHA 366
 - - - ROESY 369
 - - - TOCSY 366, 368
 - rotor 23
 - ruthenium complex, PHIP spectrum 619
- S**
- sagging behavior 456, 474
 - sample cell 69
 - concentration 80
 - preparation 67
 - spinning 74
 - tube 19, 69
 - - coaxial 69
 - sampling rate 256
 - satellite lines 49
 - satellites, ^{13}C 226 ff.
 - saturation 23
 - factor 624
 - Saupe matrix 565, 568
 - scalar coupling, *see spin-spin coupling* 43
 - scalar product, of nuclear magnetic moments 42
 - scanner, whole body 645
 - Schrödinger equation 14, 151
 - screening constant 30
 - secondary isotope effect 591
 - secular determinant 160
 - equations 161
 - selection rules 156
 - selective, inversion recovery 269
 - population inversion (SPI) 357
 - - transfer (SPT) 358
 - pulses 261
 - semimetals 437 ff.
 - self-diffusion 613
 - sensitive line 644
 - point 644
 - sensitivity 19, 26, 76, 78 ff., 364, 599
 - enhancement 617 ff.
 - test, with ethylbenzene 78
 - SELTICS (side band suppression) 573
 - pulse sequence 575
 - spectrum of tyrosin hydrochloride 575
 - shielding constant 30
 - shift correlation $^{15}\text{N}, ^1\text{H}$ 629
 - shifted sine bell 285
 - shift reagents, chiral 219
 - table 603
 - Shigemi tube 67
 - shim coils 75
 - shimming 75
 - SHR (States-Haberland-Ruben) 301
 - SI sytem (système international) 672
 - side bands 74
 - sigma, shielding or screening constant 30
 - value, calculation 31

- signal enhancement 344
 - height 36, 245
 - phase 75, 259 ff., 671
 - shape 75
 - superposition 72
 - width, *see line width*
- signal-to-noise ratio 78, 364
 - table 364
- silanes 455
- silica spectra, solid state NMR 582
- sine bell window function 285
- single coil spectrometer 19
 - quantum coherence (SQ) 307, 310
 - scan NMR 337
- silicon-29, *see also heteronuclei* 456 ff.
- soft pulses 261
- solid state NMR, *see also high-resolution solid state NMR* 22, 568 ff.
- Solomon diagram for IS 342
 - for II 343
- solvent effects 120 ff.
 - and proton exchange 73
 - aromatic 73
 - for chemical shifts 72
 - for coupling constants 72
- solvent, suppression 74, 639 ff
 - WATERGATE
 - optically active 217
 - for variable temperature measurements 82
 - highly purified 80
 - table 68, 659
 - solvent-separated ion pairs (SSIP) 586
- spatial structure 630
- spectra, high field effect 57, 510, 626
- spectral accumulation 240
 - density function 240
 - types 211, 150
- spectral analysis** 149 ff.
 - combination line 171
 - computer analysis 206
 - complex spin systems 170
 - degenerate 189, 195
 - eigenfunction 152
 - eigenstate 151
 - eigenvalue 151, 209
 - eigenvector 171, 209
 - electron on a circle 152
 - first order approximation 167
 - forbidden transition 180
 - Hamilton operator 151, 153
 - Hamilton matrix 173
 - high resolution NMR 153
 - iterative analysis 208
 - Laplace operator 152
 - LAOCOON program 207
 - lowering operator 154
 - normalized function 155
 - notion for spin systems 150
 - nuclear spin operators 154
 - orthogonal function 155
 - particle spin 181
 - product functions 156
 - quantum condition 153
 - quantum mechanical formalism 151 ff.
 - raising operator 154
 - relative intensities 151, 162
 - Schrödinger equation 151
 - secular determinant 160
 - selection rules 156
 - spin system, *see also individual entries* 42, 149
 - – A₂ 158
 - – AA'BB' 205, 666
 - – AA'XX' 192 ff.
 - – AB 164 ff.
 - – – with J = 0 157
 - – AB₂ (A₂B) 177 ff.
 - – ABX 182 ff.
 - – AX 167 ff.
 - – – calculation 155 ff.
 - – – degenerate 226
 - – general rules for 170
 - – notation for 150
 - stationary state 151, 156
 - subspectral analysis 182
 - subspectrum 182
 - transition moment 162
 - unitary transformation 174
 - variational method 158
 - virtual coupling 190
 - wave function 151, 154
 - – antisymmetric 163
 - – symmetric 163
 - X-approximation 183
- spectral density function 240
- spectrometer 16
 - schematic diagram 20, 256
 - tuning 74 ff
- spherical aromaticity 416
- SPI (selective population inversion)
 - experiment 357 ff.
 - AX system 358
 - chloroform 359
 - multiplicity and intensity of A_nX groups 360
- spin chromatography 335
- spin decoupling, *see spin-spin decoupling*
- spin diffusion 349

- spin echo experiment 248 ff., 285 ff.
 - for ^{13}C assignment (SEFT) 383 ff.
 - for coupled spin systems 286 ff.
 - PFGSTE 614, 615
 - PGSE 613
 - pulse sequence 249
 - with AX system 288
 - with pulsed gradients 613
- spin echo spectroscopy, two-dimensional, *see also J-resolved spectra*
- spin-flip method 402
- spin functions 43
 - lock 364 ff.
 - quantum number 14
 - states 14, 43
 - of A_2X_3 system 46
- spin-lattice relaxation 239 ff.
 - benzene 242, 248
 - in ^{13}C NMR 428
 - mechanism 240
- spinlock 364
 - experiments in solution 366 ff.
- spin mapping 644
- spinning side bands 74
- spin quantum number 14
 - rotation relaxation 243, 480
 - spin temperature 19
 - orientation in B_0 15
- spin-spin coupling** 41 ff
 - $^{13}\text{C}, ^{13}\text{C}$ 422
 - – Karplus curve 423
 - $^{13}\text{C}, ^1\text{H}$ 424
 - – Karplus curve 427
 - carbon-13 420 ff.
 - chemical exchange, influence of 503
 - energy of 42
 - $^1\text{H}, ^1\text{H}$ 122 ff.
 - – allenes 142
 - – allylic 141
 - – $^1\text{H}, ^2\text{H}$ (H,D) 229
 - – benzene 658
 - – benzenes, monosubstituted 655
 - – bond length dependence 130
 - – 1.3-butadiene 658
 - – cumulenes 142
 - – dihedral angle dependence (Karplus curve) 129
 - – dipolar 143
 - – direct 143
 - – electronegativity 124, 133
 - – geminal 123
 - – HCC valence angles 132
 - – homoallylic 142
 - – hybridization 123
 - – Karplus curve 229
 - – long-range 137 ff.
 - – M (W) mechanism 138
 - – magnitude 47
 - – MO model 126
 - – naphthalene 658
 - – neighboring π -bonds 124
 - – olefins 654
 - – π -mechanism 137 ff.
 - – polyacetylenes 142
 - – propenes 140
 - – saturated systems 138
 - – solvent effects 72
 - – tables 654 ff.
 - – through space 143
 - – transition metal complexes 136
 - – W (M) mechanism 138
 - – unsaturated systems 122, 133, 139
 - – vicinal 128 ff.
 - – with other nuclei 49 ff.
 - $J/\delta\nu$ ratio 56
 - magnitude 47
 - nuclei with $I = \frac{1}{2}$ 49
 - with $I > \frac{1}{2}$ 51, 664
 - of heteronuclei, *see heteronuclei*
 - of transition metals, *see heteronuclei*
 - rare nuclei 49
 - strong coupling 56
 - structural dependence 62
 - through-space 143, 454
 - virtual 190
 - weak coupling 56
 - spin-spin decoupling 58 ff., 272
 - broadband 59
 - – by CW modulation 275
 - – by pulse methods 275
 - – GARB 277
 - – MLEV 277
 - – WALTZ-16 277
 - – noise 275
 - – table 278
 - off-resonance 278
 - spin, spin relaxation, *see also relaxation* 43
 - splitting, first order 49
 - simple rules for 52
 - SPT (selective population transfer) 349, 358
 - SQ *see single quantum coherence*
 - stacked plot 284
 - standard, *see also reference, referencing* 33, 69
 - external 70
 - internal 70
 - static aggregates of organolithium compounds 465
 - stationary state 14, 151, 156

- stereochemistry, ^{13}C chemical shifts and 419
 – ^1H , ^1H coupling and 128
 Stern-Gerlach experiment 17
 steroid chemistry 72
 strong coupling 56
 structural dependence, of proton chemical shift 37, 85 ff.
 styrene oxide 66
 subspectral analysis 182
 subspectrum 182
 substituent constants 121, 652, 653, 662
 sulfur dioxide 67
 superconducting magnet, *see cryomagnet*
 supramolecular chemistry 616
 surface coils 641
 susceptibility, diamagnetic 71, 94
 – correction 71
 – exaltation 110
 – volume 70 ff.
 sweep direction 75
 sweep 21
 symmetrization 301
 syndiotactic polymers 223
- t**
- T_1 measurement 247
 t_1 noise 302
 temperature measurement 81 ff.
 – with liquid crystals 82
 tensor, chemical shift 14, 571
 testosterone, ^{13}C spectrum 380
 tetramethylsilane 33, 67
 thermal mixing (TM) 626
 thermotropic compounds 558
 three-dimensional experiment 372
 through space coupling 143, 454
 time, domain 252
 – increment 61
 – scales 281
 – sharing 259
 – signal 21
 tin-119, *see also heteronuclei* 473 ff.
 tissue investigation 641
 titration curve 93
 TOCSY spectroscopy 366
 – spectrum 2D, β -D-glucose 368
 – – 1D, β -D-glucose + α -D-glucose 370
 – one dimensional 368
 – pulse sequence, 2D 367
 Tolman angle 487
 total spin 45
 total correlation spectroscopy, *see TOCSY*
 366 ff.
- TOSS (total suppression of side bands) 573
 TPPI (time proportional phase increment) 301
trans-ethyl crotonate, spectrum 58
 transition 16
 – probability 19
 – metal complexes, ^1H , ^1H coupling 136
 – metals, *see also heteronuclei* 476 ff.
 transmission coefficient 507
 transmitter 259 ff.
 – coil 16
 transition state, transoid 533
 transverse magnetization 238
 – effect of spin-spin coupling 287
 – time-dependence 285
 – by chemical exchange 246
 – in solids 569
 – optimized spectroscopy, *see TROSY*
 – mechanism 244
 triads, in polymers 223
 – heterotactic 223
 – isotactic 223
 – syndiotactic 223
 “trial and error” method 207
 trialkyloxonium salt 526
 trimethylaluminium 550
 triphenylphosphine 574
 1,2,3- trichlorobenzene, spectrum 57
 trifluoroacetic acid 67
 [D_4]3-trimethylsilylpropionic acid 70
 triplet state 166
 tris(dipivaloylmethanato)-Eu(III) 601
 tropylium ion 89
 TROSY (transverse magnetization optimized spectroscopy) 629
 tungsten-183, *see also heteronuclei* 494 ff.
 tuning, of spectrometer 74 ff.
 two spin system 43
- two-dimensional NMR** 60, 281 ff.
- absolute value representation 285
 – amplitude modulation 282
 – anti-echo signal 325
 – axial peaks 302
 – BIRD pulse 330
 – chemical shift correlation:
 – heteronuclear, *see also individual entries*
 – – HEHAHA 366
 – – HETCOR 389
 – – HMBC 395, 397
 – – HMQC 389, 474, 566
 – – HSQC 391, 566
 – homonuclear, *see also individual entries*
 – – COLOC experiment 394

- - COSY-90 experiment 296 ff., 317
 - - COSY-45 304
 - - COSY-DQF 307, 320, 327
 - - COSY-LR 305
 - - E.COSY 630
 - coherence transfer echo 325
 - constant time experiment 395
 - contour diagram, plot 7, 284
 - cross peak 7, 60, 301
 - data improvement 269
 - detection time t_2 282
 - diagonal peak 7, 60, 301
 - echo signal 288, 325
 - evolution of operators 313
 - evolution time t_1 61, 281
 - exchange spectroscopy (EXSY) 516
 - ω_1 -decoupled COSY 329
 - filter functions 285
 - gradient enhanced spectroscopy 303, 326
 - graphical presentation 284
 - HOESY experiment 355
 - INADEQUATE experiment 331
 - Jeener experiment 296
 - J -resolved NMR, heteronuclear 372, 403
 - - homonuclear 289 ff.
 - - in solid state MAS 577
 - long-range correlation, heteronuclear 395
 - - homonuclear 305
 - low-pass filter 330
 - magnitude representation 285
 - mixing time 281
 - multiple quantum coherences 312
 - multiple quantum magic angle spinning (MQMAS) 469
 - NOESY experiment 350 ff.
 - N-type signal 325
 - P-type signal 325
 - phase 259
 - - correction 286
 - - cycles 266
 - - error, frequency-dependent 259
 - - modulation 282
 - - rule 322
 - phase-sensitive detection 300
 - preparation period 317
 - - time 381
 - principles of 2D NMR 281 ff.
 - product operator formalism 309
 - propagator 314
 - quad-images 265
 - quadrature detection 264
 - ROESY experiment 369
 - signal phase, *see phase*
 - single quantum coherences 307
 - stacked plot 284
 - t_1 noise 302
 - TOCSY experiment, 2D 366
 - - 1D 368
 - TPPI method 301, 325
 - window or weighting functions 272
 - z-filter 331
 - zero-quantum coherences 310
- u**
- unitary transformation 174
 - upfield 32
- v**
- valence tautomerism, *see also dynamic NMR* 532 ff.
 - L-valin 219
 - van-der-Waals effect 86, 114
 - variable angle sample spinning (VASS) 567
 - variable temperature 81 ff.
 - variational method 158
 - vicinal ^1H , ^1H coupling 128 ff.
 - and bond length 130
 - and bond order 132
 - and dihedral angle 129
 - and HCC valence angles 132
 - substituent effects 133
 - transition metal complexes 136
 - vinylcyclopropane 113
 - virtual coupling 190
 - volume susceptibility 70
 - measurement of 71
- w**
- Wagner–Meerwein rearrangements 548
 - WAHUHA sequence 573
 - W(M)-arrangement 138
 - WALTZ-16 277
 - WATERGATE 640
 - wave function 14, 154
 - antisymmetric 163
 - symmetric 163
 - weak coupling 56
 - weighting functions 272
 - whole-body scanner 645
 - wide-bore cryomagnets 641
 - Wiedemann's law 71
 - wiggles 75
 - window or weighting functions 272
 - word length 254

x

- X-approximation 183
- Xenon-129 NMR 621 ff.
 - chemical shift scale 621
 - in zeolite 622
 - on mesoporous silica 622
 - – EXSY spectrum 622
- m*-xylene, ^{13}C T_1 measurement 381

z

- Zeeman effect 15
- Zeeman splitting 15
- zeolite 584, 622
- zero filling 270
- zero quantum coherence 312
- z-filter 329
- zig-zag-arrangement 138