

Cumulative Subject Index for 1997¹ Volumes 124–129

A

- Absorption**
artifact-free pure-phase PFG-enhanced double-quantum-filtered COSY spectra including gradient pulse in evolution period, Ancian *et al.*, **125**, 348
lineshapes, in 2D ESR, and effects of slow motions in complex fluids, Saxena and Freed, **124**, 439
pure absorption 2D TOCSY, ROESY, and NOESY spectra, quick recording using pulsed field gradients, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
- Acquisition**
parameters, selection for NMR experiment, graphical approach, Early, Donahue, and Williams, **125**, 163
simultaneous, quadrupolar order and double-quantum ²³Na signals, Jung, Cannon, and Katz, **129**, 130
whole echo, in 2D multiple quantum MAS NMR, Brown and Wimperis, **124**, 279
- Acquisition delay**
data, application of detection–estimation scheme for noisy NMR signals, Lin *et al.*, **128**, 30
- Adiabatic decoupling**
coherence sidebands in, elimination, Bendall and Skinner, **129**, 30
reducing sidebands in, phase-cycling algorithm for, Skinner and Bendall, **124**, 474
sidebands in, effect of sweep direction, Kupče, **129**, 219
- Adiabatic demagnetization in rotating frame**
differential cross polarization spectroscopy of synthetic calcium phosphates and bone mineral, Ramanathan and Ackerman, **127**, 26
- Adiabatic pulses**
compensation for spin–spin coupling effects during, Kupče and Freeman, **127**, 36
refocusing, potential for unlimited bandwidths and excellent phase stability with, Hwang, van Zijl, and Garwood, **124**, 250
selective, optimization, Rosenfeld, Panfil, and Zur, **126**, 221
selective inversion, design using adiabatic condition, Rosenfeld, Panfil, and Zur, **129**, 115
- Adiabatic slice-selective excitation for surface coils**
RF pulse designed for, Shen and Rothman, **124**, 72
- ADRF** (*see* Adiabatic demagnetization in rotating frame)
- Adsorption**
di-*tert*-butyl nitroxide on Au(111) and NiO(111), ESR and TPD studies, evidence for long-range interactions, Katter *et al.*, **126**, 242
- Advanced method for accurate robust and efficient spectral fitting**
quantification of MRS data with use of prior knowledge, Vanhamme, van den Boogaart, and Van Huffel, **129**, 35
- ¹⁰⁷Ag
pulsed ENDOR spectroscopy at large thermal spin polarizations, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- ¹⁰⁹Ag
pulsed ENDOR spectroscopy at large thermal spin polarizations, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- ²⁷Al
chemical shielding anisotropy, Vosegaard and Jakobsen, **128**, 135
corundum, quadrupole coupling constant, magnetic field dependence, Fil-singer *et al.*, **125**, 280
2D multiple quantum MAS NMR
acquisition of whole echo, Brown and Wimperis, **124**, 279
comparison of methods, Brown and Wimperis, **128**, 42
soft-pulsed quadrupolar central transition NMR studies of ovotransferrin, Aramini, Germann, and Vogel, **129**, 111
- Alanine**
L-[1,3-¹³C₂, ¹⁵N]alanine, orientational information from REDOR sidebands, Goetz and Schaefer, **129**, 222
and glycine, substitution for tryptophan, effects on heterogeneity of gramicidin A analogs in micelles, Hinton *et al.*, **124**, 132
- Algorithms**
phase-cycling, for reducing sidebands in adiabatic decoupling, Skinner and Bendall, **124**, 474
- α -Al₂O₃
²⁷Al chemical shielding anisotropy, Vosegaard and Jakobsen, **128**, 135
- Aluminum gallium arsenide**
–GaAs heterostructures, optically detected nuclear magnetic resonance in, lineshapes, Schreiner *et al.*, **124**, 80
- AMARES** (*see* Advanced method for accurate robust and efficient spectral fitting)
- Amides**
¹⁷O chemical shifts, solvent effects: quantitative linear solvation shift relationships, Díez *et al.*, **124**, 8
proton chemical-shift anisotropy, determination in ¹⁵N-labeled proteins using ¹H CSA/¹⁵N–¹H dipolar and ¹⁵N CSA/¹⁵N–¹H dipolar cross-correlation rates, Tessari *et al.*, **127**, 128
protons, and ¹⁵N, in deuterated proteins, triple-resonance 4D correlation, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
side-chain amide protons in proteins, stereospecific assignment with H₂NCO-E.COSY, Löhr and Rüterjans, **124**, 255
- Amplitude**
modulated decoupling pulses, in liquid-state NMR, Geen and Böhlen, **125**, 376
reductions caused by off-resonance effects with CPMG pulse sequence, affecting motional analysis of biomolecules, Ross, Czisch, and King, **124**, 355
time-domain quantitation by wavelet-transform analysis, Serrai *et al.*, **124**, 20
- 4-Androsten-3,17-dione**
proton chemical-shift spectrum, Simova, Sengstschmid, and Freeman, **124**, 104
- Anisotropic interactions**
under magic-angle spinning, multidimensional solid-state NMR for correlation of, Fujiwara, Shimomura, and Akutsu, **124**, 147
- Anisotropy**
chemical shielding
²⁷Al, Vosegaard and Jakobsen, **128**, 135
spin relaxation induced by, evaluation: importance of antisymmetric component, Kowalewski and Werbelow, **128**, 144

¹ Boldface numbers indicate volume; lightface numbers indicate pagination.

- orientational, determination in glassy solids by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
- proton chemical-shift
- amide, determination in ^{15}N -labeled proteins using ^1H CSA/ ^{15}N - ^1H dipolar and ^{15}N CSA/ ^{15}N - ^1H dipolar cross-correlation rates, Tessari *et al.*, **127**, 128
- effect on MAS spectra of hydrate crystals, Tekely, **127**, 238
- Annealing
- mean-field simulated, protein heteronuclear NMR assignments using, Buchler *et al.*, **125**, 34
- Antamanide
- dihedral-angle distribution based on three-bond coupling information: polypeptide-structure determination in presence of conformational equilibria, Schmidt, **124**, 310
- $^3J_{\text{HC}}$ coupling constants, determination by 2D NMR multiplet simulation for analysis of conformational equilibria, Schmidt, **124**, 298
- Antibiotic
- peptide, degree of coupled isotopic enrichment of different positions in, NMR measurement, Miller, Egan, and Townsend, **125**, 120
- Antisymmetry
- and shielding anisotropy, effects on ^{15}N spin relaxation, Kowalewski and Werbelow, **128**, 144
- Artifacts
- convection, suppression in double-stimulated-echo diffusion experiments, Jerschow and Müller, **125**, 372
- negative edge enhancement in NMR imaging with diffusion at permeable susceptibility interfaces, Nestle, Rydyger, and Kimmich, **125**, 355
- pure absorption PFG-enhanced double-quantum-filtered COSY spectra free of, including gradient pulse in evolution period, Ancian *et al.*, **125**, 348
- AsO_4^{4-}
- as spin probe in paraelectric phase of KH_2AsO_4 , electron-nuclear dipolar relaxation, ESR study, Rakvin and Merunka, **126**, 87
- Assignment
- backbone, $^{15}\text{N}(i+1)$, $^{13}\text{C}\alpha(i)$, and $^1\text{H}\alpha(i)$ backbone resonances in $^{13}\text{C}/^{15}\text{N}$ -labeled proteins, correlation by (CO)N(CO)CAH experiment, Dijkstra *et al.*, **125**, 149
- carboxylate groups in uniformly $^{15}\text{N}/^{13}\text{C}$ -labeled proteins, 2D NMR experiments $\text{H}(\text{C})\text{CO}_2$ and HCCO_2 for, Pellecchia *et al.*, **124**, 274
- ^{13}C NMR spectra of rigid solids by 2D MAS separated-local-field spectroscopy, Pan, **124**, 1
- protein, heteronuclear NMR, method using mean-field simulated annealing, Buchler *et al.*, **125**, 34
- resonance of smaller ^{13}C -labeled biomolecules, 2D $ct\text{-HC}(\text{C})\text{H-COSY}$ for, Szyperski, Fernández, and Wüthrich, **128**, 228
- stereospecific, side-chain amide protons in proteins with $\text{H}_2\text{NCO-E.COSY}$, Löhner and Rüterjans, **124**, 255
- Atomic orbitals
- transition metals, hyperfine-coupling parameters for, Rieger, **124**, 140
- Automation
- analysis of MRS time-domain data, use of continuous regularization in, Totz *et al.*, **124**, 400
- signal class recognition by Bayesian method, use of global symmetries in, Schulte *et al.*, **129**, 165
- Averaging
- far-off-resonance, dipolar interactions in solids, Chang *et al.*, **124**, 165
- 4,4'-Azoxydianisole
- molecular motion in, ^2H double-quantum NMR spectroscopy study, Duer and Stourton, **129**, 44
- B**
- ^{10}B
- sodium borocaptate, quadrupolar relaxation of spin 3 in intermediate $\omega_0\tau_c$ regime, Baram and Bendel, **129**, 10
- ^{11}B
- multiple-quantum MAS NMR spectra of quadrupolar nuclei, indirect spin-spin coupling in, Wu *et al.*, **124**, 237
- Bandwidth
- working, approach for constructing time-symmetric adiabatic refocusing pulses with no appreciable phase distortion within, Hwang, van Zijl, and Garwood, **124**, 250
- Barium chlorate monohydrate
- crystals, MAS spectra, effect of proton chemical-shift anisotropy, Tekely, **127**, 238
- Bases
- types in ^{13}C -uniformly labeled RNAs, identification of ribose-base sequential NOEs according to, Ramachandran *et al.*, **124**, 210
- Bayesian method
- automated signal class recognition by, use of global symmetries in, Schulte *et al.*, **129**, 165
- Beads
- polymeric resin, peptides on, 2D NMR spectroscopy, Jelinek *et al.*, **125**, 185
- Benzene ring
- inner, 1,4-diphenoxybenzene, time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
- Bilayers
- oriented lipid
- cross-polarized peptide samples in, dipolar oscillations, Tian and Cross, **125**, 220
- preparation on ultrathin polymers for solid-state NMR analyses of peptide-membrane interactions, Augé *et al.*, **124**, 455
- Biofluids
- multiple- ^{13}C -labeled, ultra-high-resolved HSQC spectra, Willker, Flögel, and Leibfritz, **125**, 216
- Biological macromolecules
- pulse sequences for, integration of optimized Water-PRESS pulse sequence, Price, Hayamizu, and Arata, **126**, 256
- Biological materials
- solid-state NMR, phase-cycling schemes for multiple π -pulse sequences in, Igumenova, Mitchell, and Evans, **127**, 144
- Biological systems
- phantoms simulating, measurement of ^{23}Na T_2 and content ratio by use of multiple-quantum filtering, Jung, Cannon, and Katz, **124**, 393
- Biomolecules
- high-field NMR, ROESY with water flip back for, Fulton and Ni, **129**, 93
- motional analysis, systematic errors associated with CPMG pulse sequence affecting, Ross, Czisch, and King, **124**, 355
- smaller, ^{13}C -labeled, 2D $ct\text{-HC}(\text{C})\text{H-COSY}$ for resonance assignments, Szyperski, Fernández, and Wüthrich, **128**, 228
- Biphenyl
- deuterated, spin diffusion in single crystal, Müller, Zimmermann, and Haeberlen, **126**, 66
- BIRD
- double-SLBIRD, 2D HSQC, application of use of RF gradients in excitation sculpting, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80
- and TANGO, RF gradient sequence to eliminate uncoupled magnetization, Sodickson and Cory, **125**, 340
- Bisphenol-A polycarbonate
- doubly ^{13}C -labeled, orientational anisotropy determination by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
- Blood
- foam preparation, NMR of laser-polarized ^{129}Xe , Tseng *et al.*, **126**, 79
- Bond polarization theory
- semi-empirical approach for calculation of ^{13}C chemical-shift tensors based on, Sternberg and Prié, **125**, 8

- Bone mineral
and synthetic calcium phosphates, ADRF differential cross polarization spectroscopy, Ramanathan and Ackerman, **127**, 26
- Book reviews
Bruch, Ed., "NMR Spectroscopy Techniques," **125**, 229
Canet, "Nuclear Magnetic Resonance, Concepts and Methods," **124**, 520
Hoch and Stern, "NMR Data Processing," **124**, 520
Rao and Kemple, "NMR as a Structural Tool for Macromolecules. Current Status and Future Directions," **125**, 228
Rusling and Kumosinski, "Nonlinear Computer Modeling of Chemical and Biochemical Data," **125**, 228
Schmidt-Rohr and Wolfgang, "Multidimensional Solid-State NMR and Polymers," **125**, 229
Atta-ur-Rahman and Choudhary, "Solving Problems with NMR Spectroscopy," **125**, 228
Tycko, Ed., "Nuclear Magnetic Resonance Probes of Molecular Dynamics," **124**, 521
- Brain
human, multislice imaging of T_1 at 4.1 T, application of general approach to error estimation and optimized experiment design, Mason, Chu, and Hetherington, **126**, 18
- Breast tumors
human MCF7, dynamic contrast-enhanced imaging and analysis at high spatial resolution, Furman-Haran, Grobgedl, and Degani, **128**, 161
- Broadening
 g -strain, and exchange effects, relationship to resolution in high-field EPR spectroscopy of undiluted Cr(V) salts, $S = \frac{1}{2}$, Cage *et al.*, **124**, 495
- Brownian dynamics
computer simulations, in study of influence of nonconstant magnetic-field gradient on PFG NMR diffusion experiments, Håkansson *et al.*, **124**, 343
- Brushite
ADRF differential cross polarization spectroscopy, Ramanathan and Ackerman, **127**, 26
- Build-up curves
and decay curves, estimating cross-relaxation rates from simultaneous fits to, robust method, Najfeld *et al.*, **124**, 372
- Bulk magnetic susceptibility
in resolution of internal and external signals in NMR spectra of plant tissues, Shachar-Hill *et al.*, **127**, 17
- ^{103}Ru
solid, multinuclear experiments on, Cherryman and Harris, **128**, 21
- C
- ^{13}C
accelerated relaxation of sensitive nucleus for enhancement of signal-to-noise with time, Homer, Pery, and Palfreyman, **125**, 20
antamanide, $^3J_{\text{HC}}$ coupling constant determination by 2D NMR multiplet simulation for analysis of conformational equilibria, Schmidt, **124**, 298
broadband polarization transfer under MAS, application to total through-space-correlation NMR spectroscopy, Baldus and Meier, **128**, 172
brucine, adiabatic decoupling, effect of sweep direction on sidebands in, Kupče, **129**, 219
chemical-shift tensors, semi-empirical approach for calculation, Sternberg and Prié, **125**, 8
 $^{13}\text{CH}_3\text{I}$, elimination of coherence sidebands in adiabatic decoupling, Bendall and Skinner, **129**, 30
 ^{13}C - $\{^1\text{H}\}$ spectra of 2,2'-difluorobiphenyl in isotropic and liquid crystalline phases: general features of X part of ABX spin system, Edgar, Emsley, and Furby, **128**, 105
compensation for spin-spin coupling effects during adiabatic pulses, Kupče and Freeman, **127**, 36
constant-time HQQC experiment for protein NMR spectroscopy, Shaw *et al.*, **124**, 479
CPMAS measurements under high gas pressures, Miyoshi, Takegoshi, and Terao, **125**, 383
2D HSQC, application of use of RF gradients in excitation sculpting, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80
doubly labeled bisphenol-A polycarbonate, orientational anisotropy determination by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
enriched proteins, field dependence of J modulation in 2D NMR spectra on, measurement of dipolar contributions to $^1J_{\text{CH}}$ splittings from, Tjandra and Bax, **124**, 512
EPR hyperfine interaction in complex $[\text{Rh}(\text{CN})_6]^{4-}$ in KCl host lattice, Vugman, Giannoni, and Coelho Neto, **124**, 352
D-[1- ^{13}C , 1- ^2H]glucose complexed to *E. coli* periplasmic glucose/galactose receptor, dynamic frequency shifts, Gabel *et al.*, **128**, 101
 ^{-1}H dipolar interactions, amplification in 2D MAS NMR, and application to torsion angle determination in peptides, Hong *et al.*, **129**, 85
high-field high-speed CP-MAS heteronuclear dipolar-correlation spectroscopy of solids with frequency-switched Lee-Goldberg homonuclear decoupling, van Rossum, Förster, and de Groot, **124**, 516
interatomic distance determination by zero-quantum correlation spectroscopy under conditions of rotational resonance, Koons *et al.*, **124**, 499
labeled proteins in H_2O , doubly sensitivity-enhanced 3D HCCH-TOCSY using heteronuclear cross polarization and pulsed-field gradients, Wijmenga, Steensma, and van Mierlo, **124**, 459
linear spin systems, signs of small $J(^1\text{H}, ^{13}\text{C})$ coupling constants in, DQ/ZQ NMR experiment for determination, Otting, **124**, 503
multidimensional solid-state NMR for correlating anisotropic interactions under MAS conditions, Fujiwara, Shimomura, and Akutsu, **124**, 147
multidimensional spectrum, importing resolution into evolution dimension of, McGeorge *et al.*, **129**, 134
multiple- ^{13}C -labeled biofluids, ultra-high-resolved HSQC spectra, Wilker, Flögel, and Leibfritz, **125**, 216
multiplet splittings in paramagnetic proteins, electron spin-nuclear spin cross-correlation effects on, Ghose and Prestegard, **128**, 138
multiplicity-edited HSQC experiments, gradient-based 1D and 2D, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
and ^{15}N , labeled proteins
alanine, orientational information from REDOR sidebands, Goetz and Schaefer, **129**, 222
assignment and pH titration of carboxylate groups in, 2D NMR experiments $\text{H}(\text{C})\text{CO}_2$ and HCCO_2 for, Pellecchia *et al.*, **124**, 274
flavodoxin, side-chain amide protons in, stereospecific assignment with $\text{H}_2\text{NCO-E.COSY}$, Löhner and Rüterjans, **124**, 255
 $^{15}\text{N}(i+1)$, $^{13}\text{C}\alpha(i)$, and $^1\text{H}\alpha(i)$ backbone resonances in, correlation by $(\text{CO})\text{N}(\text{CO})\text{CAH}$ experiment, Dijkstra *et al.*, **125**, 149
relaxation mechanisms of backbone carbonyl carbons in, Allard and Härd, **126**, 48
resolution enhancement in out-and-back triple-resonance experiments applied to HCAO sequence, Baur and Kessler, **126**, 270
NMR measurement of degree of coupled isotopic enrichment of different positions in antibiotic peptide, Miller, Egan, and Townsend, **125**, 120
NMR spectra of rigid solids, assignment by 2D MAS separated-local-field spectroscopy, Pan, **124**, 1
proton decoupling in humans at 4 Tesla, half-volume coil for, Adriano and Gruetter, **125**, 178
proton-detected ^{13}C - ^{13}C double-quantum coherence, Meissner *et al.*, **124**, 245
REDOR dephasing by multiple spins in presence of molecular motion, Goetz and Schaefer, **127**, 147
relaxation, role of shielding antisymmetry, Kowalewski and Werbelow, **128**, 144

- RNAs uniformly labeled with, base types in, identification of ribose-base sequential NOEs according to, Ramachandran *et al.*, **124**, 210
- selective ^1H - ^{13}C 1D polarization-transfer schemes, sensitivity improvements, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
- selective homonuclear polarization transfer in tilted rotating frame under MAS in solids, Takegoshi, Nomura, and Terao, **127**, 206
- sensitivity- and gradient-enhanced heteronuclear coupled/decoupled HSQC-TOCSY experiments for measuring long-range heteronuclear coupling constants, Kövér, Hruby, and Uhrin, **129**, 125
- smaller biomolecules labeled with, 2D *ct*-HC(C)H-COSY for resonance assignments, Szyperski, Fernández, and Wüthrich, **128**, 228
- subspectrum of glucose in plant shoot segments: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
- 1,3,7,10-tetramethylbenzo[*c*]cinnoline, NMR study of internal rotation of mutually interacting methyl groups, Wimmer and Müller, **129**, 1
- time-reverse ODESSA experiment for rotating solids with several groups of equivalent nuclei, Reichert *et al.*, **125**, 245
- zinc acetate labeled with, 1D and 2D MAS NMR spectra of dipolar-coupled homonuclear spin- $\frac{1}{2}$ pair, Kundla *et al.*, **129**, 53
- $^{13}\text{C}^{\alpha}$
- selectively labeled peptide, selective transient heteronuclear cross relaxation in, Allard, Jarvet, and Gräslund, **124**, 97
- Calcium alginate gel
- NMR imaging with diffusion at permeable susceptibility interfaces, negative edge enhancement in, Nestle, Rydyger, and Kimmich, **125**, 355
- Calcium phosphates
- synthetic, ADRF differential cross polarization spectroscopy, Ramathan and Ackerman, **127**, 26
- Calibration
- in situ*, in quantification of maximum-entropy reconstructions, Schmieder *et al.*, **125**, 332
- Capillary
- convection in, pulsed-gradient spin-echo NMR measurements, Manz, Seymour, and Callaghan, **125**, 153
- Carbon multiplicities
- edited HSQC experiments, gradient-based 1D and 2D, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
- Carbons
- backbone carbonyl, in ^{13}C , ^{15}N -labeled protein, relaxation mechanisms in, Allard and Härd, **126**, 48
- Carbonyl groups
- backbone, carbons, in ^{13}C , ^{15}N -labeled protein, relaxation mechanisms in, Allard and Härd, **126**, 48
- ^{17}O NMR chemical shifts in, comparison of experimental and ab initio values, Jackowski, Jaszuński, and Makulski, **127**, 139
- Carboxylate groups
- in uniformly $^{15}\text{N}/^{13}\text{C}$ -labeled proteins, assignment and pH titration, 2D NMR experiments H(C)CO₂ and HCCO₂ for, Pellecchia *et al.*, **124**, 274
- Carr-Purcell-Meiboom-Gill
- associated systematic errors affecting motional analysis of biomolecules, Ross, Czisch, and King, **124**, 355
- Cavity
- double TE₁₀₄ and single TE₁₀₂ rectangular, analysis of movement of line-like samples of variable length along *x*-axis of, Mazúr, Morris, and Valko, **129**, 188
- CDCl₃
- automated shimming using field profiling, Sukumar *et al.*, **125**, 159
- Cell extracts
- glioma cells, multiple- ^{13}C -labeled, ultra-high-resolved HSQC spectra, Willker, Flögel, and Leibfritz, **125**, 216
- Cellular volume
- isolated rat heart, continuous monitoring during normothermic perfusion and ischemia, Askenasy and Navon, **124**, 42
- Chemical deposition
- silver, bridged loop-gap resonator made by, pulsed EPR with field cycling using, Sturm, Lötzer, and Voithländer, **127**, 105
- Chemical-shielding anisotropy
- ^{27}Al , Vosegaard and Jakobsen, **128**, 135
- spin relaxation induced by, evaluation: importance of antisymmetric component, Kowalewski and Werbelow, **128**, 144
- Chemical-shift anisotropy
- amide proton, determination in ^{15}N -labeled proteins using ^1H CSA/ ^{15}N - ^1H dipolar and ^{15}N CSA/ ^{15}N - ^1H dipolar cross-correlation rates, Tesari *et al.*, **127**, 128
- proton, effect on MAS spectra of hydrate crystals, Tekely, **127**, 238
- Chemical-shift imaging
- 2D ^1H , human muscle metabolites, Hu, Willcott, and Moore, **126**, 187
- fast, theoretical evaluation and comparison of methods, Pohmann, von Kienlin, and Haase, **129**, 145
- radial spectroscopic, Meininger *et al.*, **125**, 325
- Chemical-shift reagent
- intracellular Na monitoring in isolated perfused rat heart in absence of, evaluation of multiple-quantum-filtered ^{23}Na NMR in, Tauskela *et al.*, **127**, 115
- Chemical shifts
- ^{17}O
- in amides, solvent effects: quantitative linear solvation shift relationships, Díez *et al.*, **124**, 8
- in carbonyl group, comparison of experimental and ab initio values, Jackowski, Jaszuński, and Makulski, **127**, 139
- proton, methods for obtaining high-resolution spectra without spin-spin splittings, Simova, Sengstschmid, and Freeman, **124**, 104
- time-domain quantitation by wavelet-transform analysis, Serrai *et al.*, **124**, 20
- Chemical-shift tensor
- ^{13}C , semi-empirical approach for calculation, Sternberg and Prié, **125**, 8
- ^{31}P , retrieval of information for dihydrogen phosphates in presence of homonuclear ^{31}P - ^{31}P dipolar coupling, Lagier and Olivieri, **126**, 138
- Chromium(IV) salts
- undiluted, 375-GHz EPR measurements, $S = \frac{1}{2}$ system, resolution in relation to exchange effects and *g*-strain broadening, Cage *et al.*, **124**, 495
- ^{35}Cl
- spectrum of oriented maize root tips: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
- ^{37}Cl
- NMR spectra in plant tissues: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
- C_3N_4
- solid, N NMR shieldings in models for, second-nearest-neighbor effects, Tossell, **127**, 49
- ^{59}Co
- NMR of cobaltcyanide, in continuous monitoring during normothermic perfusion and ischemia, Askenasy and Navon, **124**, 42
- Cobaltcyanide
- ^{59}Co NMR, in continuous monitoring during normothermic perfusion and ischemia, Askenasy and Navon, **124**, 42
- Cog-wheel model
- nuclear-spin propagation in solids, Brüschweiler and Ernst, **124**, 122
- Coherence
- double- and quadruple-quantum, detection for spin $\frac{7}{2}$ excited by spin lock pulse sequences, Ageev, Mann, and Sanctuary, **128**, 12
- heteronuclear quadruple-quantum, constant-time experiment for protein NMR spectroscopy, Shaw *et al.*, **124**, 479
- multiple-quantum intermolecular, with intramolecular *J* coupling in solution NMR, quantum treatment of, Ahn, Warren, and Lee, **128**, 114
- proton-detected ^{13}C - ^{13}C double-quantum, Meissner *et al.*, **124**, 245

- zero-quantum, elimination of associated effects in 1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302
- Coherence sidebands
in adiabatic decoupling, elimination, Bendall and Skinner, **129**, 30
- Coherence transfer
calculation under planar vs isotropic mixing Hamiltonians and application to heteronuclear J cross-polarization experiments in solution-state NMR spectroscopy, Krishnan and Rance, **124**, 205
distortions, in rotating frame cross-relaxation spectra, origin of correlation time dependence of, Ghose, Evans, and Prestegard, **128**, 207
- Coils
birdcage
calculation of B_1 fields in three dimensions: effects of shield geometry on field strength and homogeneity, Collins *et al.*, **125**, 233
resonant modes, Leifer, **124**, 51
half-volume, for efficient proton decoupling in humans at 4 Tesla, Adriany and Gruetter, **125**, 178
planar quadrature, design using shielded-loop resonators, Stensgaard, **125**, 84
single-layer cylindrical, shielding of low-frequency magnetic interference in weak-field MRI by, Planinšič, **126**, 30
solenoid-like, producing transverse RF fields for MR imaging, Jeong *et al.*, **127**, 73
surface
adiabatic slice-selective excitation for, Shen and Rothman, **124**, 72
stray-field imaging of planar films using, Glover, McDonald, and Newling, **126**, 207
- Complete-relaxation-matrix analysis
flexible program RELAX based on, for back calculation of NOESY spectra, Görler and Kalbitzer, **124**, 177
off-resonance ROESY spectra, for DNA duplex with G–A mismatch in solution, Kuwata *et al.*, **128**, 70
- Complexed ligands
dynamic frequency shifts: D-[1- ^{13}C ,1- ^2H]glucose complexed to *E. coli* periplasmic glucose/galactose receptor, Gabel *et al.*, **128**, 101
- Computers
personal, real-time NMR imaging systems using, Kose *et al.*, **124**, 35
- (CO)N(CO)CAH experiment
correlation of $^{15}\text{N}(i+1)$, $^{13}\text{C}\alpha(i)$, and $^1\text{H}\alpha(i)$ backbone resonances in $^{13}\text{C}/^{15}\text{N}$ -labeled proteins, Dijkstra *et al.*, **125**, 149
- Conformational database potential
for refinement of NMR and X-ray structures of proteins and nucleic acids, improvements and extensions, Kuszewski, Gronenborn, and Clore, **125**, 171
- Conformational equilibria
in polypeptides
determination of $^3J_{\text{HC}}$ coupling constants in antamanide by 2D NMR multiplet simulation, Schmidt, **124**, 298
dihedral-angle distribution in antamanide based on three-bond coupling information, Schmidt, **124**, 310
- Constant- λ algorithm
in quantification of maximum-entropy reconstructions, Schmieder *et al.*, **125**, 332
- Continuous regularization
in automated analysis of MRS time-domain data, Totz *et al.*, **124**, 400
- Continuous wavelet transform
spectral line analysis and applications, Barache, Antoine, and Dereppe, **128**, 1
- Convection
artifacts produced by, suppression in double-stimulated-echo diffusion experiments, Jerschow and Müller, **125**, 372
in capillary, pulsed-gradient spin-echo NMR measurements, Manz, Seymour, and Callaghan, **125**, 153
- Cooling
thermoelectric, for NMR sample temperature control, Gregory, Claridge, and Leonard, **124**, 228
- Corrections and Additions, **125**, 231; **127**, 134; **128**, 98
- Correlation
triple resonance 4D, sequential amide protons and nitrogens-15 in deuterated proteins, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
- Correlation spectroscopy
2D *ct*- $\text{HC}(\text{C})\text{H}$ -COSY, for resonance assignments of smaller ^{13}C -labeled biomolecules, Szyperski, Fernández, and Wüthrich, **128**, 228
PFG-enhanced double-quantum-filtered pure absorption, artifact-free, including gradient pulse in evolution period, Ancian *et al.*, **125**, 348
stripe-COSY and superstripe-COSY pulse sequences, combined with selective deuteration strategy, improved measurement of ^1H – ^1H coupling constants via, Yang *et al.*, **129**, 212
zero-quantum, under rotational-resonance conditions, determination of interatomic distances by, Koons *et al.*, **124**, 499
- Correlation time
rotational, internuclear vectors in DNA duplex with G–A mismatch in solution, by complete-relaxation-matrix analysis of O-ROESY spectra, Kuwata *et al.*, **128**, 70
- Correlation time dependence
coherence transfer distortions in rotating frame cross-relaxation spectra, origin, Ghose, Evans, and Prestegard, **128**, 207
for frequency offset: selection of spin-lock transmitter position to minimize HOHAHA distortions of ROESY spectra, Chan *et al.*, **126**, 183
- Corundum
 ^{27}Al , quadrupole coupling constant, magnetic field dependence, Filsinger *et al.*, **125**, 280
- COSY (*see* Correlation spectroscopy)
- Coupling (*see also* Dipolar coupling; Quadrupole couplings; Spin–spin coupling)
hyperfine
to nucleus of arbitrary spin, electron-spin-echo envelope modulation arising from, Ponti, **127**, 87
for transition metals, atomic parameters for, Rieger, **124**, 140
across ice–water interface, observation by 2D time domain NMR, Weglarz and Peemoeller, **124**, 484
scalar, in detection of influence of deuterium on ^{15}N nucleus of side chains, Boyd *et al.*, **124**, 61
strong, effects in 1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302
- CPMG (*see* Carr–Purcell–Meiboom–Gill)
- Cross-correlation
electron spin–nuclear spin, effects on multiplet splittings in paramagnetic proteins, Ghose and Prestegard, **128**, 138
homonuclear cross-correlation cross-relaxation rates along effective field, application to dipole–dipole cross-correlation, Desvaux, **127**, 1
and spin diffusion, effect on net NOE enhancement in NMR, Madhu and Kumar, **127**, 168
- Cross-correlation rates
 ^1H CSA/ ^{15}N – ^1H dipolar and ^{15}N CSA/ ^{15}N – ^1H dipolar, in determination of amide proton chemical-shift anisotropy in ^{15}N -labeled proteins, Tessari *et al.*, **127**, 128
- Cross peaks
E.COSY-type, determination of heteronuclear coupling constants from, HMQC- and HSQC-based 2D NMR experiments: HECADÉ, Koźmiński and Nanz, **124**, 383
tilted, pure-phase homo- and heteronuclear J -spectra with, for determination of coupling constants, Koźmiński *et al.*, **125**, 193

- Cross polarization heteronuclear
J, experiments in solution-state NMR spectroscopy, application of calculation of coherence-transfer behavior under planar vs isotropic mixing Hamiltonians, Krishnan and Rance, **124**, 205
 and pulsed-field gradients, in doubly sensitivity-enhanced 3D HCCH-TOCSY of ¹³C-labeled in H₂O, Wijmenga, Steensma, and van Mierlo, **124**, 459
 in solid-state MAS NMR, combination of slow and fast RF field modulation for improvement of, Hediger *et al.*, **125**, 291
- magic-angle spinning
¹³C measurements under high gas pressures, Miyoshi, Takegoshi, and Terao, **125**, 383
 high-field high-speed ¹³C NMR heteronuclear dipolar-correlation spectroscopy of solids with frequency-switched Lee–Goldberg homonuclear decoupling, van Rossum, Förster, and de Groot, **124**, 516
 peptide samples in oriented lipid bilayers, and dipolar oscillations as function of mixing time, Tian and Cross, **125**, 220
- Cross relaxation
 effects, elimination from measurement of relaxation rates of ¹H longitudinal modes, Norwood, **125**, 265
 homonuclear cross-correlation cross-relaxation rates along effective field, application to dipole–dipole cross-correlation, Desvaux, **127**, 1
 rate estimation from simultaneous fits to build-up and decay curves, robust method for, Najfeld *et al.*, **124**, 372
 selective transient heteronuclear, in selectively ¹³C^α-labeled peptide, Allard, Jarvet, and Gräslund, **124**, 97
 and spin diffusion, in solid-state NMR, Müller, Zimmermann, and Haebleren, **126**, 66
- Cross-relaxation
 rotating-frame, coherence transfer distortions in spectra, origin of correlation time dependence, Ghose, Evans, and Prestegard, **128**, 207
- Crystals
 hydrate, MAS spectra, effect of proton chemical-shift anisotropy, Tekely, **127**, 238
- Cyclic sampling
 fresh spins for NMR signal enhancement using, Wu and Johnson, **127**, 225
- Cylindrical pore
 diffusive diffraction in, observations by pulsed-field-gradient NMR, Gibbs, **124**, 223
- D
- Data analysis
¹⁵N relaxation data, applicability of model-free approach, Korzhnev, Orekhov, and Arseniev, **127**, 184
- Decay curves
 and build-up curves, estimating cross-relaxation rates from simultaneous fits to, robust method, Najfeld *et al.*, **124**, 372
- Decomposition
 singular-value, post-acquisition solvent suppression by, Zhu, Smith, and Hua, **124**, 286
- Decoupling
 adiabatic (*see* Adiabatic decoupling)
 deuterium, and isotope dilution and variable angle sample spinning, in measurement of interproton nuclear spin dipolar couplings in liquid crystalline samples, Ciampi, De Luca, and Emsley, **129**, 207
 frequency-switched Lee–Goldberg homonuclear, high-field high-speed CP-MAS ¹³C NMR heteronuclear dipolar-correlation spectroscopy of solids with, van Rossum, Förster, and de Groot, **124**, 516
 heteronuclear spin, amplitude-modulated pulses, in liquid-state NMR, Geen and Böhlen, **125**, 376
 homonuclear broadband, NMR spectra, Zangger and Sterk, **124**, 486
 proton, in humans at 4 Tesla, half-volume coil for, Adriany and Gruetter, **125**, 178
- Dephasing
 REDOR, by multiple spins in presence of molecular motion, Goetz and Schaefer, **127**, 147
- Detection–estimation scheme
 for noisy NMR signals, applications to delayed acquisition data, Lin *et al.*, **128**, 30
- Deuteration
 selective, combined with stripe-COSY and superstripe-COSY pulse sequences, improved measurement of ¹H–¹H coupling constants via, Yang *et al.*, **129**, 212
- Deuterium
 deuterated solvents, automated shimming using field profiling, Sukumar *et al.*, **125**, 159
 NMR spectrum and *T*₁ of hydroxyl deuterons in single crystals of tropolone-*d*₁, orientation and temperature dependence: dynamic hydrogen disorder, Detken *et al.*, **126**, 95
 quadrupole couplings, solution NMR characterization of hydrogen bonds in protein by indirect measurement of, LiWang and Bax, **127**, 54
 scalar-coupled, effect on relaxation of ¹⁵N nucleus and use as probe for side-chain interactions in proteins, Boyd *et al.*, **124**, 61
- Deuterium decoupling
 and isotope dilution and variable angle sample spinning, in measurement of interproton nuclear spin dipolar couplings in liquid crystalline samples, Ciampi, De Luca, and Emsley, **129**, 207
- Deuterons
 hydroxyl, in single crystals of tropolone, NMR study: dynamic hydrogen disorder, Detken *et al.*, **126**, 95
- Diazo systems
 off-angle fast-sample-spinning NMR and self-consistent-field calculations: studies of isolated ¹⁵N–¹⁵N spin pair, Challoner, Harris, and Tossell, **126**, 1
- Di-*tert*-butyl nitroxide
 adsorption on Au(111) and NiO(111), ESR and TPD studies, evidence for long-range interactions, Katter *et al.*, **126**, 242
- Dielectric resonator
 double-stacked, for sensitive EPR measurements, Jaworski, Sienkiewicz, and Scholes, **124**, 87
- Difference spectroscopy
 NOE-enhanced *J*-resolved: method for observation of NOE from regions of spectral overlap, Grode and Mowery, **126**, 142
- Differential cross polarization spectroscopy
 ADRF, synthetic calcium phosphates and bone mineral, Ramanathan and Ackerman, **127**, 26
- Diffraction
 diffusive (*see* Diffusive diffraction)
- Diffusion
 effects in 1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302
 measurement in phantoms and tissues using SLIM localization, Yang *et al.*, **129**, 161
 measurements with centric phase-encoded turboFLASH sequence, comparison of imaging strategies for, Coremans *et al.*, **124**, 323
 at permeable susceptibility interfaces, NMR imaging with, negative edge enhancement in, Nestle, Rydyger, and Kimmich, **125**, 355
 pulsed-field gradient NMR experiments, effect of nonconstant magnetic-field gradient, Brownian-dynamics computer simulation study, Håkansson *et al.*, **124**, 343
 restricted, under generalized gradient waveforms, matrix formalism for spin echo analysis of, Callaghan, **129**, 74
 Smoluchowski drift-diffusional framework, methyl-rotor electron-spin dynamics using, Sørnes and Benetis, **125**, 52

- stimulated-echo
 suppression of convection artifacts: double-STE experiments, Jerschow and Müller, **125**, 372
 using pulsed-field gradients
 heterogeneous media, Sørland, Hafskjold, and, Herstad, **124**, 172
 short-time diffusion, Sørland, **126**, 146
 and T_1 , measurements using MR signals from laser-hyperpolarized ^{129}Xe nuclei, Patyal *et al.*, **126**, 58
 Torrey–Bloch equations in NMR study of, simple solutions, Kenkre, Fukushima, and Sheltraw, **128**, 62
- Diffusion imaging
 with hyperpolarized ^3He gas, Schmidt *et al.*, **129**, 184
- Diffusive diffraction
 in cylindrical pore, observations by pulsed-field-gradient NMR, Gibbs, **124**, 223
- 2,2'-Difluorobiphenyl
 in isotropic and liquid crystalline phases, ^{13}C – $\{^1\text{H}\}$ spectra: general features of X part of ABX spin system, Edgar, Emsley, and Furby, **128**, 105
- Dihedral-angle distribution
 in antamanide, based on three-bond coupling information: polypeptide-structure determination in presence of conformational equilibria, Schmidt, **124**, 310
- Dihydrogen phosphates
 retrieval of ^{31}P chemical-shift-tensor information in presence of homonuclear ^{31}P – ^{31}P dipolar coupling, Lagier and Olivieri, **126**, 138
- 2,6-Dimethoxynaphthalene
 high-resolution 3D magic-angle turning separated-local-field experiment, Hu *et al.*, **126**, 120
- Dimethyl sulfone
 time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
- 1,4-Diphenoxybenzene
 time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
- 2,2-Diphenyl-1-picrylhydrazyl
 as standard for high-field EPR, Krzystek *et al.*, **125**, 207
- Dipolar coupling
 amplification in 2D MAS NMR, and application to torsion angle determination in peptides, Hong *et al.*, **129**, 85
 homonuclear ^{31}P – ^{31}P , retrieval of ^{31}P chemical-shift-tensor information for dihydrogen phosphates in presence of, Lagier and Olivieri, **126**, 138
 homonuclear spin- $\frac{1}{2}$ pair: 1D and 2D MAS NMR spectra, Kundla *et al.*, **129**, 53
 interproton nuclear spin, measurement in liquid crystalline samples by combined variable angle sample spinning, isotope dilution, and deuterium decoupling, Ciampi, De Luca, and Emsley, **129**, 207
 networks, under magic-angle spinning, Geen *et al.*, **125**, 224
- Dipolar DECODER
 determination of orientational anisotropy in glassy solids, Utz *et al.*, **128**, 217
- Dipolar interactions
 electron spin–nuclear spin cross-correlation effects on multiplet splittings in paramagnetic proteins, Ghose and Prestegard, **128**, 138
 ^1H CSA/ ^{15}N – ^1H dipolar and ^{15}N CSA/ ^{15}N – ^1H dipolar cross-correlation rates, in determination of amide proton chemical-shift anisotropy in ^{15}N -labeled proteins, Tessari *et al.*, **127**, 128
 measurement of dipolar contributions to $^1J_{\text{CH}}$ splittings from magnetic-field dependence of J modulation in 2D NMR spectra, Tjandra and Bax, **124**, 512
 in solids, far-off-resonance averaging, Chang *et al.*, **124**, 165
- Dipolar oscillations
 in cross-polarized peptide samples in oriented lipid bilayers, Tian and Cross, **125**, 220
- Distortions
 coherence transfer, in rotating frame cross-relaxation spectra, origin of correlation time dependence of, Ghose, Evans, and Prestegard, **128**, 207
 HOHAHA, of ROESY spectra, selection of spin-lock transmitter position for minimization, Chan *et al.*, **126**, 183
- DNA
 duplex, with G–A mismatch in solution, complete-relaxation-matrix analysis of off-resonance ROESY spectra, Kuwata *et al.*, **128**, 70
 ^1H – ^1H coupling constants, improved measurement via stripe-COSY and superstripe-COSY pulse sequences combined with selective deuteration strategy, Yang *et al.*, **129**, 212
- Dosimetry
 radiation, by localized magnetic resonance spectroscopy, Roser, **124**, 271
- Double-quantum-filtered magnetization-transfer experiment
 elucidation of dipolar coupling networks under magic-angle spinning, Geen *et al.*, **125**, 224
- Double-quantum-filtered spectroscopy
 ^2H , discrimination between compartments in sciatic nerve by, Shinar, Seo, and Navon, **129**, 98
 PFG-enhanced artifact-free pure absorption COSY including gradient pulse in evolution period, Ancian *et al.*, **125**, 348
- Double-quantum spectroscopy
 elucidation of dipolar coupling networks under magic-angle spinning, Geen *et al.*, **125**, 224
 ^2H , for study of molecular motion in solids, Duer and Stourton, **129**, 44
 pulsed-field gradient, experiments recorded with only z gradients, reduction of residual H_2O signal, Dalvit and Böhlen, **126**, 149
- Double-quantum/zero-quantum spectroscopy
 determination of signs of small $J(^1\text{H}, ^{13}\text{C})$ coupling constants in linear spin systems, Otting, **124**, 503
- DPPH (*see* 2,2-Diphenyl-1-picrylhydrazyl)
- DQ/ZQ (*see* Double-quantum/zero-quantum spectroscopy)
- Drift diffusion
 Smoluchowski model, methyl-rotor electron-spin dynamics using, Sørnes and Benetis, **125**, 52
- Durene
 deuterated, cross relaxation in single crystal, Müller, Zimmermann, and Haerberlen, **126**, 66
- Dynamic contrast
 enhanced imaging and analysis of MCF7 human breast tumors at high spatial resolution, Furman-Haran, Grobgeld, and Degani, **128**, 161
- Dynamic frequency shifts
 caused by electron spin–nuclear spin cross-correlation effects on multiplet splittings in paramagnetic proteins, Ghose and Prestegard, **128**, 138
 complexed ligands: D- $[1-^{13}\text{C}, 1-^2\text{H}]$ glucose complexed to *E. coli* periplasmic glucose/galactose receptor, Gabel *et al.*, **128**, 101
- Dynamic nuclear polarization
 imaging in very low magnetic fields with, as noninvasive technique for oximetry, Guiberteau and Grucker, **124**, 263
- Dynamics
 Brownian, computer simulations, in study of influence of nonconstant magnetic-field gradient on PFG NMR diffusion experiments, Håkansson *et al.*, **124**, 343
 electron-spin, methyl rotor in radicals, in Smoluchowski drift-diffusional framework, Sørnes and Benetis, **125**, 52
 internal, in glassy polymer matrix detected by nitroxide spin probe, double-modulation ESR study, Rakvin and Veksli, **125**, 28
 large-linewidth solids, mapping by MARF spin-lock filter, De Luca *et al.*, **126**, 159
 molecular, torsion-angle, as tool for NMR structure calculation, Stein, Rice, and Brünger, **124**, 154
 spin, 1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302

Dynamic studies

T_1 measurement using snapshot-FLASH MRI, Jivan *et al.*, **127**, 65

E

Echo (*see* Spin echoes)

E.COSY

H_2 NCO-E.COSY method for stereospecific assignment of side-chain amide protons in proteins, Löhr and Rüterjans, **124**, 255

measurement of J_{HH} coupling constants, application of spin-state-selective excitation, Meissner, Duus, and Sørensen, **128**, 92

type cross peaks, determination of heteronuclear coupling constants from, HMQC- and HSQC-based 2D NMR experiments: HECADE, Koźmiński and Nanz, **124**, 383

Edge enhancement

negative, in NMR imaging with diffusion at permeable susceptibility interfaces, Nestle, Rydyger, and Kimmich, **125**, 355

Editorials

change in Editorship, **124**, vii

Effective field

homonuclear cross-correlation cross-relaxation rates along, application to dipole–dipole cross-correlation, Desvaux, **127**, 1

Electron–nuclear dipolar interaction

ESR study of END relaxation for AsO_4^{4-} spin probe in paraelectric phase of KH_2AsO_4 , Rakvin and Merunka, **126**, 87

Electron–nuclear double resonance

pulsed experiments at large thermal spin polarizations, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199

X-band pulsed, study of ^{57}Fe -substituted sodalite: effect of zero-field splitting, Vardi *et al.*, **126**, 229

Electron paramagnetic resonance

analysis of movement of line-like samples of variable sample length along x -axis of double TE_{104} and single TE_{102} rectangular cavity, Mazúr, Morris, and Valko, **129**, 188

atomic hyperfine-coupling parameters for transition metals, Rieger, **124**, 140

^{13}C hyperfine interaction in complex $[Rh(CN)_6]^{4-}$ in KCl host lattice, Vugman, Giannoni, and Coelho Neto, **124**, 352

double-modulation, study of internal dynamics in glassy polymer matrix detected by nitroxide spin probe, Rakvin and Vekslı, **125**, 28

double-stacked dielectric resonator for, Jaworski, Sienkiewicz, and Scholes, **124**, 87

electron–nuclear dipolar relaxation for AsO_4^{4-} spin probe in paraelectric phase of KH_2AsO_4 , Rakvin and Merunka, **126**, 87

high-field, DPPH as standard for, Krzystek *et al.*, **125**, 207

internal motion of methyl fragment in radicals, simulation using Smoluchowski drift diffusion model, Sørnes and Benetis, **125**, 52

longitudinally detected, *in vivo* measurements at microwave regions of 300, 700, and 900 MHz in rats treated with nitroxide radical, Yokoyama *et al.*, **129**, 201

multifrequency 2D Fourier transform: X/Ku-band spectrometer, Borbat, Crepeau, and Freed, **127**, 155

pulsed (*see* Pulsed electron paramagnetic resonance)

–STM results, validity, demonstration with real-time response and phase-sensitive detection, Manassen, **126**, 133

375-GHz measurements on undiluted Cr(V) salts, $S = \frac{1}{2}$ system, resolution in relation to exchange effects and g -strain broadening, Cage *et al.*, **124**, 495

and TPD, studies of adsorption of di-*tert*-butyl nitroxide on Au(111) and NiO(111), evidence for long-range interactions, Katter *et al.*, **126**, 242

X-band, study of unusual center in X-irradiated zircon at 10 K, Claridge, Sutton, and Tennant, **125**, 107

Electron spin

–nuclear spin cross-correlation effects, on multiplet splittings in paramagnetic proteins, Ghose and Prestegard, **128**, 138

Electron-spin-echo envelope modulation

from hyperfine coupling to nucleus of arbitrary spin, Ponti, **127**, 87

ENDOR (*see* Electron–nuclear double resonance)

Error estimation

and optimized experiment design, general approach applied to multislice imaging of T_1 in human brain at 4.1 T, Mason, Chu, and Hetherington, **126**, 18

Errors

with CPMG pulse sequence, affecting motional analysis of biomolecules, Ross, Czisch, and King, **124**, 355

systematic, associated with off-resonance oscillations in T_2 measurements, removal, Czisch, King, and Ross, **126**, 154

Erythromycin A

tin derivative, application of optimal detection of weak $^nJ(^1H-^{119}Sn)$ couplings by gradient-enhanced 1D and 2D HMQC, Martins *et al.*, **124**, 218

ESR (*see* Electron paramagnetic resonance)

Evolution dimension

multidimensional NMR spectrum, importing resolution into, McGeorge *et al.*, **129**, 134

Exchange effects

and g -strain broadening, effects on resolution in high-field EPR spectroscopy of undiluted Cr(V) salts, $S = \frac{1}{2}$, Cage *et al.*, **124**, 495

Excitation (*see* Selective excitation)

Excitation sculpting

application to construction of singly and doubly selective 1D NMR experiments, Gradwell, Kogelberg, and Frenkiel, **124**, 267

use of RF gradients in, with application to 2D HSQC, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80

F

 ^{19}F

delayed acquisition data, application of detection–estimation scheme for noisy NMR signals, Lin *et al.*, **128**, 30

and ^{119}Sn , solid organotin fluorides, multinuclear experiments, Cherryman and Harris, **128**, 21

Far-off-resonance conditions

averaging of dipolar interactions in solids, Chang *et al.*, **124**, 165

Fast low-angle shot

snapshot, dynamic T_1 measurement using, Jivan *et al.*, **127**, 65

Fast-sample-spinning spectroscopy

off-magic-angle spinning, isolated $^{15}N-^{15}N$ spin pair in 5-methyl-2-diazobenzenesulfonic acid hydrochloride, Challoner, Harris, and Tosell, **126**, 1

Fast spectroscopic imaging

fast chemical shift imaging methods, theoretical evaluation and comparison, Pohmann, von Kienlin, and Haase, **129**, 145

Fast spiral magnetic resonance imaging

with trapezoidal gradients, Duyn and Yang, **128**, 130

Fat

and water, protons, relative concentrations and relaxation times, single-scan imaging technique for measurement of, Ma *et al.*, **125**, 92

FAWSETS

flow-driven arterial water stimulation with elimination of tissue signal, Marro, **124**, 240

 ^{57}Fe

substituted sodalite, X-band pulsed ENDOR study: effect of zero-field splitting, Vardi *et al.*, **126**, 229

Field cycling

pulsed EPR with, using bridged loop–gap resonator made by chemical deposition of silver, Sturm, Lötzer, and Voitländer, **127**, 105

- Field mapping
 B_0 field, without pulsed gradients, projection-reconstruction spectroscopic imaging for, Gregory, **129**, 173
- Field profiling
 automated shimming for deuterated solvents using, Sukumar *et al.*, **125**, 159
- Field stabilization
 and ^1H NMR spectroscopy, in 24.6 T resistive magnet, Soghomonian *et al.*, **125**, 212
- Field strength
 and homogeneity, B_1 fields in birdcage coil, effects of shield geometry, Collins *et al.*, **125**, 233
- Films
 planar, stray-field imaging using surface coil, Glover, McDonald, and Newling, **126**, 207
- Filter
 MARF spin-lock, slow dynamics mapping of large-linewidth solids by, De Luca *et al.*, **126**, 159
- Filtering
 double-quantum
 generation and elimination of intersequence stimulated echo in, mathematical analysis, Jung and Katz, **124**, 232
 and Jeener–Broecker sequence, ^{23}Na , in simultaneous acquisition and separation of quadrupolar and double-quantum signals, Jung, Cannon, and Katz, **129**, 130
 multiple-quantum, ^{23}Na , measurement of T_2 and content ratio of ^{23}Na in phantoms simulating biological systems, Jung, Cannon, and Katz, **124**, 393
- FLASH (*see* Fast low-angle shot)
- Flavodoxin
 side-chain amide protons in, stereospecific assignment with $\text{H}_2\text{NCO-E.COSY}$, Lohr and Rüterjans, **124**, 255
- Flip angles
 arbitrary, biselective and independent rotations with, for I and I{S} spin systems, novel pulse sequence element for, Briand and Sørensen, **125**, 202
- Flip back
 water, ROESY sequence for high-field NMR of biomolecules, Fulton and Ni, **129**, 93
- Flow
 driven arterial water stimulation with elimination of tissue signal, Marro, **124**, 240
 evaluation, pulse sequences based on self-refocused RF and interleaved spiral readout, Takahashi, Li, and Stødkilde-jørgensen, **126**, 127
- Flow wave
 propagation velocity, rapid MR measurement, *in vitro* validation Kraft *et al.*, **126**, 103
- Fluid distributions
 in fractured systems, NMR spectroscopic techniques for characterization, Chang *et al.*, **126**, 213
- Fluids
 complex, effects of slow motions, absorption lineshapes in 2D ESR and, Saxena and Freed, **124**, 439
- Foam
 blood, NMR of laser-polarized ^{129}Xe , Tseng *et al.*, **126**, 79
- Fourier transform spectroscopy
 interlaced, application to echo-planar spectroscopic imaging, Metzger and Hu, **125**, 166
 multifrequency 2D ESR: X/Ku-band spectrometer, Borbat, Crepeau, and Freed, **127**, 155
 NMR experimental-parameter selection, graphical approach, Early, Donahue, and Williams, **125**, 163
- Fractures
 in porous media, characterization with NMR spectroscopic techniques, Chang *et al.*, **126**, 213
- Free induction decay
 truncated multidimensional, procedure for extraction of constant-evolution-frequency data from, McGeorge *et al.*, **129**, 134
- Frequencies
 in NMR, signs of, Levitt, **126**, 164
- Fresh spins
 for NMR signal enhancement, through programmed sample translation cycles, Wu and Johnson, **127**, 225

G

- ^{71}Ga
 optical detection of nuclear magnetic resonances of GaAs/AlGaAs heterostructures, lineshapes obtained, Schreiner *et al.*, **124**, 80
- Gallium arsenide
 –AlGaAs heterostructures, optically detected nuclear magnetic resonance in, lineshapes, Schreiner *et al.*, **124**, 80
- Gas pressure
 high, ^{13}C CPMAS measurements under, Miyoshi, Takegoshi, and Terao, **125**, 383
- Gels
 Ca-alginate, NMR imaging with diffusion at permeable susceptibility interfaces, negative edge enhancement in, Nestle, Rydyger, and Kim-mich, **125**, 355
- Glasses
 solid, orientational anisotropy determination by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
- Glucose
 D-[1- ^{13}C , 1- ^2H]-labeled, complexed to *E. coli* periplasmic glucose/galactose receptor, dynamic frequency shifts, Gabel *et al.*, **128**, 101
- Glucose/galactose receptor
E. coli periplasmic, D-[1- ^{13}C , 1- ^2H]glucose complexed to, dynamic frequency shifts, Gabel *et al.*, **128**, 101
- Glycine
 and alanine, substitution for tryptophan, effects on heterogeneity of gramicidin A analogs in micelles, Hinton *et al.*, **124**, 132
- Gold
 Au(111), and NiO(111), adsorption of di-*tert*-butyl nitroxide, ESR and TPD studies: evidence for long-range interactions, Katter *et al.*, **126**, 242
- Gradients (*see also* Pulsed-field gradients)
 B_1 , fast NMR imaging with, Raulet *et al.*, **124**, 259
 continuously oscillating, 4D ^1H and ^{23}Na imaging using, Star-Lack *et al.*, **124**, 420
 electric-field, interaction with nuclear quadrupole moment, magnetic field dependence, Filsinger *et al.*, **125**, 280
 nonconstant, effect on PFG NMR diffusion experiments, Brownian-dynamics computer simulation study, Håkansson *et al.*, **124**, 343
 radiofrequency-field
 in modification of BIRD/TANGO sequences to eliminate uncoupled magnetization, Sodickson and Cory, **125**, 340
 use in excitation sculpting, with application to 2D HSQC, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80
 spiral readout, and self-refocused RF, pulse sequence for flow evaluation based on, Takahashi, Li, and Stødkilde-jørgensen, **126**, 127
 trapezoidal, fast spiral MRI with, Duyn and Yang, **128**, 130
 z , PFG DQ experiments recorded with, reduction of residual H_2O signal, Dalvit and Böhlen, **126**, 149
- Gradient selection
 ^1H – ^{13}C 1D polarization-transfer schemes with, sensitivity improvement, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
- Gradient sequence
 radiofrequency, BIRD/TANGO, to eliminate uncoupled magnetization, Sodickson and Cory, **125**, 340

Gramicidin A

$^{15}\text{N}_{1,3,5,7}$ -labeled, cross-polarized samples in oriented lipid bilayers, dipolar oscillations in, Tian and Cross, **125**, 220

Gramicidin A analogs

in micelles, heterogeneity, effects of alanine and glycine substitution for tryptophan, Hinton *et al.*, **124**, 132

in SDS micelles, relative motion of indole ring of tryptophans in, proton T_1 , T_2 , and NOE study, Hinton and Washburn-McCain, **125**, 259

H

 ^2H

double-quantum-filtered spectroscopy, discrimination between compartments in sciatic nerve by, Shinar, Seo, and Navon, **129**, 98

double-quantum NMR spectroscopy for study of molecular motion in solids, Duer and Stourton, **129**, 44

NMR spectroscopy in 24.6 T resistive magnet, Soghomonian *et al.*, **125**, 212

solid-state NMR analyses of peptide–membrane interactions, preparation of oriented lipid bilayer on ultrathin polymers for, Augé *et al.*, **124**, 455

spectrum from maize shoot segments: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17

Hard-sphere approximation

dimer formation, in determination of oligomeric state of proteins in solution from pulsed-field-gradient self-diffusion coefficient measurements, Krishnan, **124**, 468

HCACO sequence

resolution enhancement in out-and-back triple-resonance experiments applied to, Baur and Kessler, **126**, 270

HD

impurities, in solid para- H_2 , theory of multiple NMR spin echoes of, Kisvarsanyi and Sullivan, **127**, 192

 ^3He

hyperpolarized, diffusion imaging with, Schmidt *et al.*, **129**, 184

Heart

human, dynamic T_1 measurement using snapshot-FLASH MRI, Jivan *et al.*, **127**, 65

human, imaging

at 1.5, 3, and 4 T, intrinsic signal-to-noise ratio in, Wen *et al.*, **125**, 65

B_1 field distribution and intrinsic signal-to-noise ratio in, simulation as function of static magnetic field, Singerman *et al.*, **125**, 72

rat

isolated, intracellular volume, continuous monitoring during normothermic perfusion and ischemia, Askenasy and Navon, **124**, 42

isolated perfused in absence of chemical-shift reagent, monitoring of intracellular Na content, multiple-quantum-filtered ^{23}Na NMR in, Tauskela *et al.*, **127**, 115

Heterogeneous media

diffusion measurements in, stimulated-echo method using pulsed-field gradients, Sørland, Hafskjold, and Herstad, **124**, 172

NMR signal in, weak-diffusion theory of, Jensen and Chandra, **126**, 193

Heteronuclear correlation

high-resolution, between quadrupolar and spin- $\frac{1}{2}$ nuclei, using multiple-quantum MAS, Wang, De Paul, and Bull, **125**, 364

multiple-quantum

based 3D maximum-quantum correlation spectroscopy, Liu *et al.*, **129**, 67

gradient-enhanced 1D and 2D, optimal detection of weak ^1H – ^{119}Sn couplings by, application to tin derivative of erythromycin A, Martins *et al.*, **124**, 218

and HSQC, based 2D NMR experiments, for determination of heteronuclear coupling constants from E.COSY-type cross peaks: HECADE, Koźmiński and Nanz, **124**, 383

single-quantum

2D, application of use of RF gradients in excitation sculpting, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80

gradient-based 1D and 2D multiplicity-edited experiments, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274

and HMQC, based 2D NMR experiments, for determination of heteronuclear coupling constants from E.COSY-type cross peaks: HECADE, Koźmiński and Nanz, **124**, 383

measurement of degree of coupled isotopic enrichment of different positions in antibiotic peptide, Miller, Egan, and Townsend, **125**, 120

and TOCSY, sensitivity- and gradient-enhanced coupled/decoupled experiments for measuring long-range heteronuclear coupling constants, Kövér, Hruby, and Uhrin, **129**, 125

ultra-high-resolved HSQC spectra of multiple- ^{13}C -labeled biofluids, Willker, Flögel, and Leibfritz, **125**, 216

Heteronuclear couplings from ASSCI-domain experiments with E.COSY-type cross peaks

HECADE: HMQC- and HSQC-based 2D NMR experiments for determination of heteronuclear coupling constants, Koźmiński and Nanz, **124**, 383

Heteronuclear dipolar-correlation spectroscopy

high-field high-speed CP-MAS ^{13}C -NMR, of solids, with frequency-switched Lee–Goldberg homonuclear decoupling, van Rossum, Förster, and de Groot, **124**, 516

Heteronuclear Hartmann–Hahn transfer

with different bandwidths for spins I and S: *kin* HEHAHA, Carlomagno, Luy, and Glaser, **126**, 110

Heteronuclear J cross-polarization

experiments in solution-state NMR spectroscopy, application of calculation of coherence-transfer behavior under planar vs isotropic mixing Hamiltonians, Krishnan and Rance, **124**, 205

Heteronuclear multidimensional nuclear magnetic resonance

protein assignments using mean-field simulated annealing, Buchler *et al.*, **125**, 34

Heteronuclear spectroscopy

pure-phase J -spectra with tilted cross peaks, for determination of coupling constants, Koźmiński *et al.*, **125**, 193

Heterostructures

GaAs/AlGaAs, lineshapes of optically detected nuclear magnetic resonance in, Schreiner *et al.*, **124**, 80

High-field spectroscopy

biomolecules, ROESY with water flip back for, Fulton and Ni, **129**, 93

EPR, potential utility of DPPH as standard for, Krzystek *et al.*, **125**, 207

high-resolution, sample-induced RF perturbations in, Crozier *et al.*, **126**, 39

High-resolution spectroscopy

high-field, sample-induced RF perturbations in, Crozier *et al.*, **126**, 39

liposomes, using MAS NMR, intermediate-size vesicles, Traikia *et al.*, **125**, 140

MAS probe for, shimming, Sodickson and Cory, **128**, 87

on-axis shims for, fast automatic adjustment, Shen and Rothman, **127**, 229

3D magic-angle turning separated-local-field experiment, Hu *et al.*, **126**, 120

HMQC (*see* Heteronuclear correlation, multiple-quantum)

HOHAHA effects

coherence transfer distortions of ROESY spectra from, origin of correlation time dependence of, Ghose, Evans, and Prestegard, **128**, 207

distortions of ROESY spectra from, selection of spin-lock transmitter position for minimization, Chan *et al.*, **126**, 183

Homogeneity

and field strength, B_1 fields in birdcage coil, effects of shield geometry, Collins *et al.*, **125**, 233

Homonuclear spectroscopy

- cross-correlation cross-relaxation rates along effective field, application to dipole–dipole cross-correlation, Desvaux, **127**, 1
- 1D and 2D MAS NMR spectra of dipolar-coupled homonuclear spin- $\frac{1}{2}$ pair, Kundla *et al.*, **129**, 53
- pure-phase *J*-spectra with tilted cross peaks, for determination of coupling constants, Koźmiński *et al.*, **125**, 193

HQQC (see Coherence, heteronuclear quadruple-quantum)

HSQC (see Heteronuclear correlation, single-quantum)

Hydrate

- crystals, MAS spectra, effect of proton chemical-shift anisotropy, Tekely, **127**, 238

Hydrogen bonding effects

- nitrogen NMR shielding of 1,2,4,5-tetrazine, Witanowski *et al.*, **124**, 127

Hydrogen bonds

- in protein, solution NMR characterization by indirect measurement of deuterium quadrupole couplings, LiWang and Bax, **127**, 54

Hydrogen disorder

- dynamic, in solid tropolone: single-crystal NMR study of hydroxyl deuterons, Detken *et al.*, **126**, 95

Hydroxyapatite

- ADRF differential cross polarization spectroscopy, Ramanathan and Ackerman, **127**, 26

Hydroxyl

- deuterons, in single crystals of tropolone, NMR study: dynamic hydrogen disorder, Detken *et al.*, **126**, 95

Hyperfine coupling

- to nucleus of arbitrary spin, electron-spin-echo envelope modulation arising from, Ponti, **127**, 87
- for transition metals, atomic parameters for, Rieger, **124**, 140

Hyperfine interaction

- absolute sign determination: pulsed ENDOR spectroscopy at large thermal spin polarizations, Bennebroek and Schmidt, **128**, 199
- ^{13}C , in complex $[\text{Rh}(\text{CN})_6]^{4-}$ in KCl host lattice, EPR study, Vugman, Giannoni, and Coelho Neto, **124**, 352

Hyperpolarized nuclei

- ^{129}Xe , T_1 and diffusion measurements using MR signals from, Patyal *et al.*, **126**, 58

I

Ice

- water interface, coupling across, observation by 2D time domain NMR, Weglarz and Peemoeller, **124**, 484

Imaging

chemical-shift

- 2D ^1H , human muscle metabolites, Hu, Willcott, and Moore, **126**, 187
- radial spectroscopic, Meininger *et al.*, **125**, 325
- compact MRI magnet design for, by stochastic optimization, Crozier and Doddrell, **127**, 233

- diffusion, with hyperpolarized ^3He gas, Schmidt *et al.*, **129**, 184

- with diffusion at permeable susceptibility interfaces, negative edge enhancement in, Nestle, Rydyger, and Kimmich, **125**, 355

- dynamic contrast-enhanced, and analysis, MCF7 human breast tumors at high spatial resolution, Furman-Haran, Grobgeld, and Degani, **128**, 161

- dynamic nuclear polarization, in very low magnetic fields, as noninvasive technique for oximetry, Guiberteau and Grucker, **124**, 263

- echo-planar spectroscopic, application of interlaced Fourier transform, Metzger and Hu, **125**, 166

- fast chemical shift, theoretical evaluation and comparison of methods, Pohmann, von Kienlin, and Haase, **129**, 145

- fast NMR, with B_1 gradients, Raulet *et al.*, **124**, 259

- fast spiral MRI with trapezoidal gradients, Duyn and Yang, **128**, 130

- four-dimensional ^1H and ^{23}Na , using continuously oscillating gradients, Star-Lack *et al.*, **124**, 420

human cardiac

- at 1.5, 3, and 4 T, intrinsic signal-to-noise ratio in, Wen *et al.*, **125**, 65

- B_1 field distribution and intrinsic signal-to-noise ratio in, simulation as function of static magnetic field, Singerman *et al.*, **125**, 72

- multislice, T_1 in human brain at 4.1 T, application of general approach to error estimation and optimized experiment design, Mason, Chu, and Hetherington, **126**, 18

- ^{17}O -decoupled proton MR spectroscopy, in tissue model, Stolpen, Reddy, and Leigh, **125**, 1

- projection-reconstruction, for B_0 field plotting and shimming without pulsed gradients, Gregory, **129**, 173

- radial spectroscopic, Meininger *et al.*, **125**, 325

- real-time NMR, systems using personal computers, Kose *et al.*, **124**, 35

- single-scan technique for measurement of relative concentrations of fat and water protons and transverse relaxation times, Ma *et al.*, **125**, 92

- snapshot-FLASH, dynamic T_1 measurement using, Jivan *et al.*, **127**, 65
- solenoid-like coil producing transverse RF fields for, Jeong *et al.*, **127**, 73

- solid rocket propellants at 14.1 T, Maas, Merwin, and Cory, **129**, 105

- solid-state, large-linewidth solids: slow dynamics mapping by MARF spin-lock filter, De Luca *et al.*, **126**, 159

- strategies for diffusion measurements with centric phase-encoded turboFLASH sequence, comparison, Coremans *et al.*, **124**, 323

- stray-field, of planar films, using surface coil, Glover, McDonald, and Newling, **126**, 207

- 2D rotating-frame NQR, Robert and Pusiol, **127**, 109

- weak-field MRI, low-frequency magnetic interference in, shielding by single-layer cylindrical coil, Planinšič, **126**, 30

Immunoglobulin

- integration of optimized Water-PRESS pulse sequence for, Price, Hayamizu, and Arata, **126**, 256

Impurities

- HD, in solid para- H_2 , theory of multiple NMR spin echoes of, Kisvarsanyi and Sullivan, **127**, 192

Inductance

- mutual, in bird-cage resonator, Tropp, **126**, 9

Inhomogeneity

- magnetic field, effect on T_2 of quadrupolar nuclei, measurement by multiple-quantum-filtered NMR, Eliav *et al.*, **128**, 82

Interatomic distances

- determination by zero-quantum correlation spectroscopy under rotational-resonance conditions, Koons *et al.*, **124**, 499

Interfaces

- ice–water, coupling across, observation by 2D time domain NMR, Weglarz and Peemoeller, **124**, 484

- permeable susceptibility, NMR imaging with diffusion at, negative edge enhancement in, Nestle, Rydyger, and Kimmich, **125**, 355

Interference

- low-frequency magnetic, shielding in weak-field MRI by single-layer cylindrical coil, Planinšič, **126**, 30

Interference effects

- elimination in 1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302

Interleukin-2

- NMR spectroscopy, constant-time HQQC experiment for, Shaw *et al.*, **124**, 479

Inversion-recovery experiments

- water, intensity jumping and beating due to radiation damping, Chen, Mao, and Ye, **124**, 490

- Ischemia
and perfusion, normothermic, continuous monitoring of intracellular volumes in isolated rat heart during, Askenasy and Navon, **124**, 42
- Isotope dilution
and variable angle sample spinning and deuterium decoupling, in measurement of interproton nuclear spin dipolar couplings in liquid crystalline samples, Ciampi, De Luca, and Emsley, **129**, 207
- Isotopic enrichment
coupled, of different positions in antibiotic peptide, NMR measurement, Miller, Egan, and Townsend, **125**, 120
- Isotropic mixing Hamiltonian
versus planar Hamiltonian, coherence-transfer calculation under, and application to heteronuclear *J* cross-polarization experiments in solution-state NMR spectroscopy, Krishnan and Rance, **124**, 205
- Isotropic solvents
and liquid crystalline solvents, ^{13}C - $\{^1\text{H}\}$ spectra of 2,2'-difluorobiphenyl in: X part of ABX spin system, Edgar, Emsley, and Furby, **128**, 105
- J
- J*-coupling (*see* Spin-spin coupling)
- Jeener-Broeckaert sequence
and double-quantum filtering, ^{23}Na , in simultaneous acquisition and separation of quadrupolar and double-quantum signals, Jung, Cannon, and Katz, **129**, 130
- J*-resolved difference spectroscopy
NOE-enhanced: observation of NOE from regions of spectral overlap, Grode and Mowery, **126**, 142
- J* spectroscopy
two-dimensional, based methods for obtaining proton chemical-shift spectra, Simova, Sengstschmid, and Freeman, **124**, 104
- K
- KH_2AsO_4
paraelectric phase, AsO_4^{3-} spin probe in, ESR study of electron-nuclear dipolar relaxation, Rakvin and Merunka, **126**, 87
- kin* sequences
HEHAHA: heteronuclear Hartmann-Hahn transfer with different bandwidths for spins I and S, Carlomagno, Luy, and Glaser, **126**, 110
- Ku band
multifrequency 2D Fourier transform ESR X/Ku-band spectrometer, Borbat, Crepeau, and Freed, **127**, 155
- L
- Laser-polarized nuclei
 ^{129}Xe , NMR in blood foam, Tseng *et al.*, **126**, 79
- Latex coating
stray-field imaging using surface coil, Glover, McDonald, and Newling, **126**, 207
- Linear prediction combined with singular-value decomposition
automated analysis of MRS time-domain data with, use of continuous regularization in, Totz *et al.*, **124**, 400
- Lineshape
absorption, in 2D ESR, and effects of slow motions in complex fluids, Saxena and Freed, **124**, 439
Gauss-Lorentz, accurate numerical approximation to, Grivet, **125**, 102
NMR, modeling using logspline density functions, Raz, Fernandez, and Gillespie, **127**, 173
optically detected nuclear magnetic resonance in GaAs/AlGaAs heterostructures, Schreiner *et al.*, **124**, 80
- Lipids
oriented bilayers
cross-polarized peptide samples in, dipolar oscillations, Tian and Cross, **125**, 220
preparation on ultrathin polymers for solid-state NMR analyses of peptide-membrane interactions, Augé *et al.*, **124**, 455
- Liposomes
high-resolution spectra using MAS NMR, intermediate-size vesicles, Traikia *et al.*, **125**, 140
- Liquid crystalline samples
interproton nuclear spin dipolar couplings in, measurement by combined variable angle sample spinning, isotope dilution, and deuterium decoupling, Ciampi, De Luca, and Emsley, **129**, 207
- Liquid crystalline solvents
and isotropic solvents, ^{13}C - $\{^1\text{H}\}$ spectra of 2,2'-difluorobiphenyl in: X part of ABX spin system, Edgar, Emsley, and Furby, **128**, 105
- Liquids
NMR, amplitude-modulated decoupling pulses in, Geen and Böhlen, **125**, 376
- Localized spectroscopy
radiation dosimetry by, Roser, **124**, 271
SLIM, diffusion measurement in phantoms and tissues using, Yang *et al.*, **129**, 161
- Logspline density
functions, modeling NMR lineshapes using, Raz, Fernandez, and Gillespie, **127**, 173
- Longitudinally detected electron spin resonance
in vivo measurements at microwave regions of 300, 700, and 900 MHz in rats treated with nitroxide radical, Yokoyama *et al.*, **129**, 201
- Longitudinal modes
 ^1H , measurement of relaxation rates, Norwood, **125**, 265
- Lung
wet/dry ratio and T_1 and T_2 distributions, ^1H NMR measurements, Estilaei *et al.*, **124**, 410
- Lysozyme
integration of optimized Water-PRESS pulse sequence for, Price, Hayamizu, and Arata, **126**, 256
- M
- Macromolecules
biological, pulse sequences for, integration of optimized Water-PRESS pulse sequence, Price, Hayamizu, and Arata, **126**, 256
- Magic angle in rotating frame
spin-lock filter, slow dynamics mapping of large-linewidth solids by, De Luca *et al.*, **126**, 159
- Magic-angle spinning
broadband polarization transfer under, application to total through-space-correlation NMR spectroscopy, Baldus and Meier, **128**, 172
correlating anisotropic interactions under, multidimensional solid-state NMR for, Fujiwara, Shimomura, and Akutsu, **124**, 147
-cross polarization
 ^{13}C measurements under high gas pressures, Miyoshi, Takegoshi, and Terao, **125**, 383
high-field high-speed ^{13}C NMR heteronuclear dipolar-correlation spectroscopy of solids with frequency-switched Lee-Goldberg homonuclear decoupling, van Rossum, Förster, and de Groot, **124**, 516
solid-state, improved CP in, combination of slow and fast RF field modulation for, Hediger *et al.*, **125**, 291
dipolar coupling networks under, Geen *et al.*, **125**, 224
high-resolution probe, shimming, Sodickson and Cory, **128**, 87
high-resolution spectra of liposomes using, intermediate-size vesicles, Traikia *et al.*, **125**, 140
hydrate crystals, influence of proton chemical-shift anisotropy, Tekely, **127**, 238
multiple-quantum
developments for spin- $\frac{3}{2}$ nuclei, Duer and Stourton, **124**, 189
high-resolution heteronuclear correlation between quadrupolar and spin- $\frac{1}{2}$ nuclei using, Wang, De Paul, and Bull, **125**, 364

- 2D, quadrupolar nuclei
 acquisition of whole echo, Brown and Wimperis, **124**, 279
 comparison of methods, Brown and Wimperis, **128**, 42
- multiple-quantum NMR spectra of quadrupolar nuclei, indirect spin–spin coupling in, Wu *et al.*, **124**, 237
- 1D and 2D, NMR spectra of dipolar-coupled homonuclear spin- $\frac{1}{2}$ pair, Kundla *et al.*, **129**, 53
- quartz crystal temperature sensor for, Simon, **128**, 194
- selective homonuclear polarization transfer in tilted rotating frame, Takegoshi, Nomura, and Terao, **127**, 206
- slow spinning conditions, spinning sidebands arising from tightly *J*-coupled spin pairs, Wu *et al.*, **124**, 366
- 2D, coupling amplification in, and application to torsion angle determination in peptides, Hong *et al.*, **129**, 85
- Magic-angle-spinning separated-local-field spectroscopy
 2D, assignment of ^{13}C NMR spectra of rigid solids by, Pan, **124**, 1
- Magic-angle turning
 high-resolution 3D separated-local-field experiment using, Hu *et al.*, **126**, 120
- Magnesium pyrophosphate
 phosphorus dipolar coupling networks under magic-angle spinning, Geen *et al.*, **125**, 224
- Magnetic equivalence
 between nuclei of spin greater than $\frac{1}{2}$ in presence of relaxation, Szymański, **127**, 199
- Magnetic field (*see also* Gradients; Pulsed-field gradients)
 B_0 field plotting and shimming without pulsed gradients, projection-reconstruction spectroscopic imaging for, Gregory, **129**, 173
 dependence of *J* modulation in 2D NMR spectra on, measurement of dipolar contributions to $^1J_{\text{CH}}$ splittings from, Tjandra and Bax, **124**, 512
 dependence of nuclear quadrupole–electric-field gradient interaction on, Filsinger *et al.*, **125**, 280
 inhomogeneity, effect on T_2 of quadrupolar nuclei, measurement by multiple-quantum-filtered NMR, Eliav *et al.*, **128**, 82
 static, simulation of B_1 field distribution and intrinsic signal-to-noise ratio in cardiac MRI as function of, Singerman *et al.*, **125**, 72
 very low, dynamic nuclear polarization imaging in, as noninvasive technique for oximetry, Guiberteau and Grucker, **124**, 263
- Magnetic-field gradient (*see* Gradients; Pulsed-field gradients)
- Magnetic susceptibility
 bulk, in resolution of internal and external signals in NMR spectra of plant tissues, Shachar-Hill *et al.*, **127**, 17
 NMR imaging with diffusion at permeable susceptibility interfaces, negative edge enhancement in, Nestle, Rydyger, and Kimmich, **125**, 355
- Magnetization
 uncoupled, RF gradient BIRD/TANGO sequence for elimination of, Sodickson and Cory, **125**, 340
- Magnetization-transfer experiment
 elucidation of dipolar coupling networks under magic-angle spinning, Geen *et al.*, **125**, 224
- Magnets
 compact MRI, design by stochastic optimization, Crozier and Doddrell, **127**, 233
 24.6 T resistive, field stabilization and ^2H NMR spectroscopy in, Soghomonian *et al.*, **125**, 212
- MARF (*see* Magic angle in rotating frame)
- Matrix formalism
 for spin echo analysis of restricted diffusion under generalized gradient waveforms, Callaghan, **129**, 74
- Maximum-entropy reconstructions
 quantification, Schmieder *et al.*, **125**, 332
- Maximum-quantum correlation HMQC NMR spectroscopy
 3D, description, Liu *et al.*, **129**, 67
- Mechanically detected magnetic resonance
 at room temperature and normal pressure, Schaff and Veeman, **126**, 200
- Meetings and Announcements, **125**, 232, 385; **126**, 158, 287; **127**, 137, 241; **128**, 99, 233; **129**, 109, 224
- Megestrol acetate
 NOE-enhanced *J*-resolved difference spectroscopy: observation of NOE from regions of spectral overlap, Grode and Mowery, **126**, 142
- Membranes
 –peptide interactions, solid-state NMR analyses, preparation of oriented lipid bilayer on ultrathin polymers for, Augé *et al.*, **124**, 455
- Mes $_3$ SnF
 solid, multinuclear experiments on, Cherryman and Harris, **128**, 21
- Metabolites
 human muscle, 2D ^1H chemical-shift imaging, Hu, Willcott, and Moore, **126**, 187
- Metals
 transition, atomic hyperfine-coupling parameters for, Rieger, **124**, 140
- 5-Methyl-2-diazobenzenesulfonic acid hydrochloride
 isolated ^{15}N – ^{15}N spin pair, off-angle fast-sample-spinning NMR and self-consistent-field calculations, Challoner, Harris, and Tossell, **126**, 1
- Methyl groups
 mutually interacting, internal rotation, ^{13}C NMR study, Wimmer and Müller, **129**, 1
- Methyl rotor
 electron-spin dynamics in Smoluchowski drift-diffusional framework, Sørnes and Benetis, **125**, 52
- Micelles
 gramicidin A analogs in, heterogeneity, effects of alanine and glycine substitution for tryptophan, Hinton *et al.*, **124**, 132
 SDS, tryptophans in gramicidin analogs in, relative motion of indole ring, proton T_1 , T_2 , and NOE study, Hinton and Washburn-McCain, **125**, 259
- Mixing sequences
kin HEHAHA: heteronuclear Hartmann–Hahn transfer with different bandwidths for spins I and S, Carlomagno, Luy, and Glaser, **126**, 110
- Model-free approach
 applicability: ^{15}N relaxation data analysis, Korzhnev, Orekhov, and Arseniev, **127**, 184
- Modulation
 decoupling pulse amplitude, in liquid-state NMR, Geen and Böhlen, **125**, 376
J, magnetic-field dependence in 2D NMR spectra, measurement of dipolar contributions to $^1J_{\text{CH}}$ splittings from, Tjandra and Bax, **124**, 512
 RF field, combination of slow and fast, for improved cross polarization in solid-state MAS NMR, Hediger *et al.*, **125**, 291
- Molecular diffusion (*see* Diffusion)
- Molecular dynamics
 torsion-angle, as tool for NMR structure calculation, Stein, Rice, and Brünger, **124**, 154
- Motion
 molecular
 REDOR dephasing by multiple spins in presence of, Goetz and Schaefer, **127**, 147
 in solids, ^2H double-quantum NMR spectroscopy for study of, Duer and Stourton, **129**, 44
 relative, indole ring of tryptophans in gramicidin analogs incorporated into SDS micelles, ^1H T_1 , T_2 , and NOE study, Hinton and Washburn-McCain, **125**, 259
 slow, in complex fluids, absorption lineshapes in 2D ESR and, Saxena and Freed, **124**, 439
- Motional analysis
 biomolecules, systematic errors associated with CPMG pulse sequence affecting, Ross, Czisch, and King, **124**, 355

- Movement
 line-like samples of variable length along x -axis of double TE₁₀₄ and single TE₁₀₂ rectangular cavity, analysis, Mazúr, Morris, and Valko, **129**, 188
- Multidimensional spectroscopy
 E.COSY-type measurement of J_{HH} coupling constants, application of spin-state-selective excitation, Meissner, Duus, and Sørensen, **128**, 92
 evolution dimension, importing resolution into, McGeorge *et al.*, **129**, 134
 pure-phase, by reference-frequency shift, Venkata Raman and Chandrakumar, **125**, 188
 solid-state, for correlating anisotropic interactions under MAS conditions, Fujiwara, Shimomura, and Akutsu, **124**, 147
 triple resonance 4D correlation of sequential amide protons and nitrogens-15 in deuterated proteins, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
- Multifrequency electron spin resonance
 2D Fourier transform: X/Ku-band spectrometer, Borbat, Crepeau, and Freed, **127**, 155
- Multiple-quantum-filtered spectroscopy
 magnetic field inhomogeneity effect on T_2 of quadrupolar nuclei measured by, Eliav *et al.*, **128**, 82
²³Na, in monitoring of intracellular Na in isolated perfused rat heart in absence of chemical-shift reagent, Tauskela *et al.*, **127**, 115
- Multiple-quantum spectroscopy
 MAS
 high-resolution heteronuclear correlation between quadrupolar and spin- $\frac{1}{2}$ nuclei using, Wang, De Paul, and Bull, **125**, 364
 quadrupolar nuclei, indirect spin-spin coupling in, Wu *et al.*, **124**, 237
 for spin- $\frac{3}{2}$ nuclei, developments, Duer and Stourton, **124**, 189
 2D MAS, quadrupolar nuclei
 acquisition of whole echo, Brown and Wimperis, **124**, 279
 comparison of methods, Brown and Wimperis, **128**, 42
- Multiplets
 2D NMR, simulation, determination of $^3J_{\text{HC}}$ coupling constants in antamanide by, for analysis of conformational equilibria, Schmidt, **124**, 298
- Multiplet splittings
 in paramagnetic proteins, electron spin-nuclear spin cross-correlation effects on, Ghose and Prestegard, **128**, 138
- Multiplicity-edited experiments
 HSQC, gradient-based 1D and 2D, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
- Muscle
 biomedical magnetic resonance spectroscopy, application of wavelet-transform analysis, Serrai *et al.*, **124**, 20
 human, metabolites, 2D ¹H chemical-shift imaging, Hu, Willcott, and Moore, **126**, 187
- N
- ¹⁴N
 nitrate and ammonia subspectra of oriented maize root tips: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
 nitrogen NMR shielding of 1,2,4,5-tetrazine, hydrogen bonding and solvent polarity effects, Witanowski *et al.*, **124**, 127
 sodium nitroprusside, quadrupole coupling constant, magnetic field dependence, Filsinger *et al.*, **125**, 280
- ¹⁵N
 and amide protons, in deuterated proteins, triple-resonance 4D correlation, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
 and ¹³C, labeled proteins
 alanine in, orientational information from REDOR sidebands, Goetz and Schaefer, **129**, 222
 assignment and pH titration of carboxylate groups in, 2D NMR experiments H(C)CO₂ and HCCO₂ for, Pellicchia *et al.*, **124**, 274
 flavodoxin, side-chain amide protons in, stereospecific assignment with H₂NCO-E.COSY, Löhr and Rüterjans, **124**, 255
¹⁵N($i+1$), ¹³C α (i), and ¹H α (i) backbone resonances in, correlation by (CO)N(CO)CAH experiment, Dijkstra *et al.*, **125**, 149
 relaxation mechanisms of backbone carbonyl carbons in, Allard and Härd, **126**, 48
 resolution enhancement in out-and-back triple-resonance experiments applied to HACO sequence, Baur and Kessler, **126**, 270
 -¹H dipolar interactions, amplification in 2D MAS NMR, and application to torsion angle determination in peptides, Hong *et al.*, **129**, 85
 isolated ¹⁵N-¹⁵N spin pair in 5-methyl-2-diazobenzenesulfonic acid hydrochloride, off-angle fast-sample-spinning NMR and self-consistent-field calculations, Challoner, Harris, and Tossell, **126**, 1
¹⁵N_{1,3,5,7}-labeled gramicidin A, cross-polarized samples in oriented lipid bilayers, dipolar oscillations in, Tian and Cross, **125**, 220
 NMR measurement of degree of coupled isotopic enrichment of different positions in antibiotic peptide, Miller, Egan, and Townsend, **125**, 120
 NMR spectra in plant tissues: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
 proteins labeled with, amide proton chemical-shift anisotropy determination using ¹H CSA/¹⁵N-¹H dipolar and ¹⁵N CSA/¹⁵N-¹H dipolar cross-correlation rates, Tessari *et al.*, **127**, 128
 RAP 17-97, E.COSY-type measurement of J_{HH} coupling constants, application of spin-state-selective excitation, Meissner, Duus, and Sørensen, **128**, 92
 relaxation, effect of scalar-coupled deuterium and use as probe for side-chain interactions in proteins, Boyd *et al.*, **124**, 61
 relaxation data analysis, applicability of model-free approach, Korzhnev, Orekhov, and Arseniev, **127**, 184
 robust method for estimating cross-relaxation rates from simultaneous fits to build-up and decay curves, Najfeld *et al.*, **124**, 372
 second-nearest-neighbor effects on N NMR shieldings in models for solid Si₃N₄ and C₃N₄, Tossell, **127**, 49
 spin relaxation, effects of shielding anisotropy and antisymmetry, Kowalewski and Werbelow, **128**, 144
 2D NMR spectroscopy of peptides on beads, Jelinek *et al.*, **125**, 185
 2D spectra with partial overlap, measurement of relaxation rates from, Mishra *et al.*, **125**, 358
 uniformly labeled protein, ¹H $T_{1\rho}$ measurement with heteronuclear 2D spectroscopy, Almeida and Opella, **124**, 509
- ²³Na
 and ¹H, 4D imaging using continuously oscillating gradients, Star-Lack *et al.*, **124**, 420
 multiple-quantum-filtered NMR
 magnetic field inhomogeneity effect on T_2 of quadrupolar nuclei measured by, Eliav *et al.*, **128**, 82
 in monitoring of intracellular Na in isolated perfused rat heart in absence of chemical-shift reagent, Tauskela *et al.*, **127**, 115
 multiple-quantum MAS NMR for spin- $\frac{3}{2}$ nuclei, developments, Duer and Stourton, **124**, 189
 simultaneous acquisition of quadrupolar order and double-quantum signals, Jung, Cannon, and Katz, **129**, 130
 spectrum of maize root segments: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
 T_2 and content ratio, measurement in phantoms simulating biological systems by use of multiple-quantum filtering, Jung, Cannon, and Katz, **124**, 393

- 2D multiple quantum MAS NMR
 acquisition of whole echo, Brown and Wimperis, **124**, 279
 comparison of methods, Brown and Wimperis, **128**, 42
- Negative edge enhancement
 in NMR imaging with diffusion at permeable susceptibility interfaces, Nestle, Rydyger, and Kimmich, **125**, 355
- Nerves
 sciatic, compartments in, discrimination by ^2H double-quantum-filtered NMR, Shinar, Seo, and Navon, **129**, 98
- Nickel monoxide
 NiO(111), and Au(111), adsorption of di-*tert*-butyl nitroxide, ESR and TPD studies: evidence for long-range interactions, Katter *et al.*, **126**, 242
- Nitrogen shieldings
 in models for solid Si_3N_4 and C_3N_4 , second-nearest-neighbor effects, Tossell, **127**, 49
 1,2,4,5-tetrazine, hydrogen bonding and solvent polarity effects, Witowski *et al.*, **124**, 127
- Nitroxide radical
 rats treated with, *in vivo* longitudinally detected ESR measurements at microwave regions of 300, 700, and 900 MHz, Yokoyama *et al.*, **129**, 201
- Nitroxide spin probe
 internal dynamics in glassy polymer matrix detected by, double-modulation ESR study, Rakvin and Veksli, **125**, 28
- Noble gases
 as relaxation agents, Hitchens and Bryant, **124**, 227
- NOE (*see* Nuclear Overhauser effect)
- NOESY (*see* Nuclear Overhauser effect spectroscopy)
- Noise
 chemical, in biomedical magnetic resonance spectroscopy, application of wavelet-transform analysis, Serrai *et al.*, **124**, 20
 detection–estimation scheme for, applications to delayed acquisition data, Lin *et al.*, **128**, 30
 method for estimating parameters of noisy MRS signals: AMARES, Vanhamme, van den Boogaart, and Van Huffel, **129**, 35
 spectral, uncertainties in relaxation analysis of 2D NOE arising from, investigation, Likić and Prendergast, **124**, 200
- Nonlinear stimulated echoes
 experiments demonstrating, Ardelean *et al.*, **124**, 506
 multiple, Ardelean *et al.*, **127**, 217
- NQR (*see* Nuclear-quadrupole resonance)
- Nuclear Overhauser effect
 net, in NMR, effect of spin diffusion and cross correlation, Madhu and Kumar, **127**, 168
 observation from regions of spectral overlap: NOE-enhanced *J*-resolved difference spectroscopy, Grode and Mowery, **126**, 142
- Nuclear Overhauser effect spectroscopy
 back calculation of data with RELAX program based on complete-relaxation-matrix formalism, Görler and Kalbitzer, **124**, 177
 $\{^1\text{H}\}$ - ^{13}C , 1,3,7,10-tetramethylbenzo[*c*]cinnoline: internal rotation of mutually interacting methyl groups, Wimmer and Müller, **129**, 1
 –HQQC, constant-time experiment for protein NMR, Shaw *et al.*, **124**, 479
 identification of ribose-base sequential NOEs according to base types in uniformly ^{13}C -labeled RNAs, Ramachandran *et al.*, **124**, 210
 method for simulation of spectra, Allard, Helgstrand, and Hård, **129**, 19
 1D, using pulsed-field gradients, Stott *et al.*, **125**, 302
 1D gradient-enhanced, and 1D ge-TOCSY, proton chemical-shift correlation with full sensitivity using, Uhrin and Barlow, **126**, 248
 relative motion of indole ring of tryptophans in gramicidin analogs incorporated into SDS micelles, Hinton and Washburn-McCain, **125**, 259
 and ROESY and TOCSY, pure absorption 2D spectra, quick recording using pulsed field gradients, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
- 2D, relaxation analysis, investigation of uncertainties arising from spectral noise, Likić and Prendergast, **124**, 200
- Nuclear-Overhauser-enhanced *J*-resolved difference spectroscopy
 method for observation of NOE from regions of spectral overlap, Grode and Mowery, **126**, 142
- Nuclear quadrupole moment
 interaction with electric-field gradient, magnetic field dependence, Filsinger *et al.*, **125**, 280
- Nuclear-quadrupole resonance
 2D rotating-frame imaging, Robert and Pusiol, **127**, 109
- Nuclear spin
 –electron spin cross-correlation effects, on multiplet splittings in paramagnetic proteins, Ghose and Prestegard, **128**, 138
- Nuclei (*see also* Quadrupolar nuclei)
 with arbitrary spin, electron-spin-echo envelope modulation arising from hyperfine coupling to, Ponti, **127**, 87
 equivalent, rotating solids with several groups of, time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
 hyperpolarized, ^{129}Xe , T_1 and diffusion measurements using MR signals from, Patyal *et al.*, **126**, 58
 laser-polarized, ^{129}Xe , NMR in blood foam, Tseng *et al.*, **126**, 79
 sensitive, accelerated relaxation for enhancement of signal-to-noise with time, Homer, Perry, and Palfreyman, **125**, 20
 spin- $\frac{1}{2}$ and quadrupolar, high-resolution heteronuclear correlation using multiple-quantum MAS, Wang, De Paul, and Bull, **125**, 364
 spin greater than $\frac{1}{2}$, magnetic equivalence in presence of relaxation, Szymański, **127**, 199
 spin- $\frac{3}{2}$, developments in multiple-quantum MAS NMR for, Duer and Stourton, **124**, 189
- Nucleic acids
 NMR and X-ray structures, conformational database potential for refinement of, improvements and extensions, Kuszewski, Gronenborn, and Clore, **125**, 171

O

 ^{17}O

- chemical shifts in amides: quantitative linear solvation shift relationships, Diez *et al.*, **124**, 8
 chemical shifts in carbonyl group, comparison of experimental and ab initio values, Jackowski, Jaszunski, and Makulski, **127**, 139
- ^{17}O -decoupled spectroscopy
 proton NMR, and imaging, in tissue model, Stolpen, Reddy, and Leigh, **125**, 1
- ODESSA (*see* One-dimensional exchange spectroscopy by sideband alternation)
- Off-magic-angle spinning
 fast-sample-rotation, isolated ^{15}N – ^{15}N spin pair in 5-methyl-2-diazobenzene-sulfonic acid hydrochloride, Challoner, Harris, and Tossell, **126**, 1
- Off-resonance effects
 associated with CPMG pulse sequence, affecting motional analysis of biomolecules, Ross, Czisch, and King, **124**, 355
 systematic errors associated with off-resonance oscillations in T_2 measurements, removal, Czisch, King, and Ross, **126**, 154
- Off-resonance irradiation effect
 in steady-state NMR saturation transfer, Baguet and Roby, **128**, 149
- Off-resonance ROESY (*see* Rotating-frame Overhauser effect spectroscopy, off-resonance)
- Oligomerization
 proteins in solution, determination from pulsed-field-gradient self-diffusion coefficient measurements, comparison of experimental, theoretical, and hard-sphere approximated values, Krishnan, **124**, 468

- One-dimensional exchange spectroscopy by sideband alternation
time-reverse, for rotating solids with several groups of equivalent nuclei, Reichert *et al.*, **125**, 245
- One-dimensional spectroscopy
gradient-based multiplicity-edited HSQC experiments, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
gradient-enhanced proton chemical-shift correlation with full sensitivity, Uhrin and Barlow, **126**, 248
NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302
selective ^1H - ^{13}C polarization-transfer schemes, sensitivity improvements, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
singly and doubly selective, application of excitation sculpting to construction of, Gradwell, Kogelberg, and Frenkiel, **124**, 267
time-of-flight: *in vitro* validation of rapid MR measurement of wave velocity, Kraft *et al.*, **126**, 103
- Optical detection of nuclear magnetic resonances
GaAs/AlGaAs heterostructures, lineshapes obtained, Schreiner *et al.*, **124**, 80
- Optimization
experiment design, and error estimation, general approach applied to multislice imaging of T_1 in human brain at 4.1 T, Mason, Chu, and Hetherington, **126**, 18
sampling strategies for measurement of relaxation times in proteins, Jones, **126**, 283
selective adiabatic inversion pulses: design using adiabatic condition, Rosenfeld, Panfil, and Zur, **129**, 115
selective adiabatic pulses, Rosenfeld, Panfil, and Zur, **126**, 221
stochastic, compact MRI magnet design by, Crozier and Doddrell, **127**, 233
Water-PRESS pulse sequence, and integration into pulse sequences for study of biological macromolecules, Price, Hayamizu, and Arata, **126**, 256
- Organotin fluorides
solid, multinuclear experiments on, Cherryman and Harris, **128**, 21
- Oriental anisotropy
determination in glassy solids by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
- Oriental information
in solids, from REDOR sidebands, Goetz and Schaefer, **129**, 222
- Oscillations
dipolar, in cross-polarized peptide samples in oriented lipid bilayers, Tian and Cross, **125**, 220
off-resonance, associated systematic errors in T_2 measurements, removal, Czisch, King, and Ross, **126**, 154
- Out-and-back experiments
triple-resonance, resolution enhancement applied to HCACO sequence, Baur and Kessler, **126**, 270
- Overlap
partial, 2D spectra with, measurement of relaxation rates from, Mishra *et al.*, **125**, 358
spectral, regions of, observation of NOE: NOE-enhanced J -resolved difference spectroscopy, Grode and Mowery, **126**, 142
- Ovotransferrin
soft-pulsed ^{27}Al quadrupolar central transition NMR studies, Aramini, Germann, and Vogel, **129**, 111
- Oximetry
dynamic nuclear polarization imaging in very low magnetic fields as noninvasive technique for, Guiberteau and Grucker, **124**, 263
- chemical-shift-tensor information, retrieval for dihydrogen phosphates in presence of homonuclear ^{31}P - ^{31}P dipolar coupling, Lagier and Olivieri, **126**, 138
elucidation of dipolar coupling networks under magic-angle spinning, Geen *et al.*, **125**, 224
MRS time-domain data, automated analysis, use of continuous regularization in, Totz *et al.*, **124**, 400
NMR spectra in plant tissues: use of bulk magnetic susceptibility to resolve internal and external signals, Shachar-Hill *et al.*, **127**, 17
phase-cycling schemes for multiple π -pulse sequences, comparative studies, Igumenova, Mitchell, and Evans, **127**, 144
spinning sidebands in slow-MAS NMR spectra arising from tightly J -coupled spin pairs, Wu *et al.*, **124**, 366
- Paint films
stray-field imaging using surface coil, Glover, McDonald, and Newling, **126**, 207
- Paraelectric phase
 KH_2AsO_4 , AsO_4^{4-} spin probe in, ESR study of electron-nuclear dipolar relaxation, Rakvin and Merunka, **126**, 87
- Paraffin
amorphous polymer matrices detected by nitroxide spin probe, internal dynamics in, double-modulation ESR study, Rakvin and Vekslis, **125**, 28
- Parahydrogen
solid, theory of multiple NMR spin echoes of HD impurities in, Kisvarsanyi and Sullivan, **127**, 192
- Paramagnetic center
unusual, in X-irradiated zircon at 10 K, X-band EPR study, Claridge, Sutton, and Tennant, **125**, 107
- Paramagnetic proteins
multiplet splittings in, electron spin-nuclear spin cross-correlation effects on, Ghose and Prestegard, **128**, 138
- Peptides
antibiotic, degree of coupled isotopic enrichment of different positions in, NMR measurement, Miller, Egan, and Townsend, **125**, 120
on beads, 2D NMR spectroscopy, Jelinek *et al.*, **125**, 185
cross-polarized samples in oriented lipid bilayers, dipolar oscillations in, Tian and Cross, **125**, 220
-membrane interactions, solid-state NMR analyses, preparation of oriented lipid bilayer on ultrathin polymers for, Augé *et al.*, **124**, 455
selectively $^{13}\text{C}^{\alpha}$ -labeled, selective transient heteronuclear cross relaxation in, Allard, Jarvet, and Gräslund, **124**, 97
torsion angle determination, application of coupling amplification in 2D MAS NMR, Hong *et al.*, **129**, 85
- Perfusion
and ischemia, normothermic, continuous monitoring of intracellular volumes in isolated rat heart during, Askenasy and Navon, **124**, 42
measurement by FAWSETS: flow-driven arterial water stimulation with elimination of tissue signal, Marro, **124**, 240
- Perturbations
RF, sample-induced, in high-field high-resolution NMR spectroscopy, Crozier *et al.*, **126**, 39
- PFG (*see* Pulsed-field gradients)
- Phantoms
semisolid tissue, ^{17}O -decoupled proton MR spectroscopy and imaging in, Stolpen, Reddy, and Leigh, **125**, 1
simulating biological systems, measurement of ^{23}Na T_2 and content ratio by use of multiple-quantum filtering, Jung, Cannon, and Katz, **124**, 393
and tissues, diffusion measurement using SLIM localization, Yang *et al.*, **129**, 161
- Phase correction
signal perturbed by eddy currents, using continuous wavelet transform, Barache, Antoine, and Dereppe, **128**, 1

P

 ^{31}P

- ADRF differential cross polarization spectroscopy of synthetic calcium phosphates and bone mineral, Ramanathan and Ackerman, **127**, 26

- Phase cycling
 algorithm, for reducing sidebands in adiabatic decoupling, Skinner and Bendall, **124**, 474
 schemes, for multiple π -pulse sequences, comparative studies, Igumenova, Mitchell, and Evans, **127**, 144
- Phase distortion
 broadband adiabatic refocusing without, Hwang, van Zijl, and Garwood, **124**, 250
- Phases
 arbitrary, biselective and independent rotations with, for I and I{S} spin systems, novel pulse sequence element for, Briand and Sørensen, **125**, 202
 in NMR, signs of, Levitt, **126**, 164
 time-domain quantitation by wavelet-transform analysis, Serrai *et al.*, **124**, 20
- Phase-sensitive detection
 and real-time response, demonstration of validity of ESR–STM results, Manassen, **126**, 133
- pH titration
 carboxylate groups in uniformly $^{15}\text{N}/^{13}\text{C}$ -labeled proteins, 2D NMR experiments $\text{H}(\text{C})\text{CO}_2$ and HCCO_2 for, Pellecchia *et al.*, **124**, 274
- Planar coupling Hamiltonian
versus isotropic mixing Hamiltonian, coherence-transfer calculation under, and application to heteronuclear J cross-polarization experiments in solution-state NMR spectroscopy, Krishnan and Rance, **124**, 205
- Plants
Ancistrocladus heyneanus, metabolites in, radial spectroscopic imaging, Meininger *et al.*, **125**, 325
 tissues, internal and external signals in NMR spectra, use of bulk magnetic susceptibility to resolve, Shachar-Hill *et al.*, **127**, 17
- Polarizations
 large thermal spin, pulsed ENDOR spectroscopy at, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- Polarization transfer
 broadband, under MAS, application to total through-space-correlation NMR spectroscopy, Baldus and Meier, **128**, 172
 selective ^1H – ^{13}C 1D, sensitivity improvements, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
 selective homonuclear, in tilted rotating frame under MAS in solids, Takegoshi, Nomura, and Terao, **127**, 206
- Polybutadiene
 amorphous polymer matrices detected by nitroxide spin probe, internal dynamics in, double-modulation ESR study, Rakvin and Vekšli, **125**, 28
- Polyisobutylene
 amorphous polymer matrices detected by nitroxide spin probe, internal dynamics in, double-modulation ESR study, Rakvin and Vekšli, **125**, 28
- Polymer matrix
 glassy, detected by nitroxide spin probe, internal dynamics in, double-modulation ESR study, Rakvin and Vekšli, **125**, 28
- Polymers
 solution, convectional flow in capillary, pulsed-gradient spin-echo NMR measurements, Manz, Seymour, and Callaghan, **125**, 153
 ultrathin, preparation of oriented lipid bilayer on, for solid-state NMR analyses of peptide–membrane interactions, Augé *et al.*, **124**, 455
- Poly(methyl methacrylate)
 amorphous polymer matrices detected by nitroxide spin probe, internal dynamics in, double-modulation ESR study, Rakvin and Vekšli, **125**, 28
- Polypeptides
 conformational equilibria
 determination of $^3J_{\text{HC}}$ coupling constants in antamanide by 2D NMR multiplet simulation, Schmidt, **124**, 298
 dihedral-angle distribution in antamanide based on three-bond coupling information, Schmidt, **124**, 310
- Polystyrene
 ^{13}C CPMAS measurements under high gas pressures, Miyoshi, Takegoshi, and Terao, **125**, 383
- Pore
 cylindrical, diffusive diffraction in, observations by pulsed-field-gradient NMR, Gibbs, **124**, 223
- Porous media
 fracture characterization with NMR spectroscopic techniques, Chang *et al.*, **126**, 213
 pulsed-field gradient stimulated-echo diffusion measurements
 ethane in saturated H-ZSM5 zeolite, Sørland, Hafskjold, and, Herstad, **124**, 172
 short-time, Sørland, **126**, 146
- Post-acquisition methods
 solvent suppression, by singular-value decomposition, Zhu, Smith, and Hua, **124**, 286
- Potassium chloride
 host lattice, ^{13}C EPR hyperfine interaction in complex $[\text{Rh}(\text{CN})_6]^{4-}$ in, Vugman, Giannoni, and Coelho Neto, **124**, 352
- Powder averaging
 efficient, in solid-state NMR, REPULSION approach, Bak and Nielsen, **125**, 132
- Preservation of equivalent pathways
 sensitivity improvement
 gradient-based 1D and 2D multiplicity-edited HSQC experiments, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
 selective ^1H – ^{13}C polarization-transfer schemes, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
- Pressure
 normal, and room temperature, mechanically detected magnetic resonance at, Schaff and Veeman, **126**, 200
- Progressive saturation experiment
 STEAM, T_1 measurement in, effect of long echo times, Knight-Scott and Li, **126**, 266
- Projection reconstruction
 spectroscopic imaging, for B_0 field plotting and shimming without pulsed gradients, Gregory, **129**, 173
- Propellants
 rocket, solid, imaging at 14.1 T, Maas, Merwin, and Cory, **129**, 105
- Proteins
 ^{13}C , ^{15}N -labeled, relaxation mechanisms for backbone carbonyl carbons in, Allard and Härd, **126**, 48
 ^{13}C -labeled, in H_2O , doubly sensitivity-enhanced 3D HCCH–TOCSY using heteronuclear cross polarization and pulsed-field gradients, Wijmenga, Steensma, and van Mierlo, **124**, 459
 $^{13}\text{C}/^{15}\text{N}$ -labeled, $^{15}\text{N}(i+1)$, $^{13}\text{C}\alpha(i)$, and $^1\text{H}\alpha(i)$ backbone resonances in, correlation by (CO)N(CO)CAH experiment, Dijkstra *et al.*, **125**, 149
 deuterated, sequential amide protons and nitrogens-15 in, triple-resonance 4D correlation, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
 heteronuclear NMR assignments using mean-field simulated annealing, Buchler *et al.*, **125**, 34
 hydrogen bonds in, solution NMR characterization by indirect measurement of deuterium quadrupole couplings, LiWang and Bax, **127**, 54
 measurement of relaxation times, optimal sampling strategies for, Jones, **126**, 283
 ^{15}N -labeled, amide proton chemical-shift anisotropy determination using ^1H CSA/ ^{15}N – ^1H dipolar and ^{15}N CSA/ ^{15}N – ^1H dipolar cross-correlation rates, Tessari *et al.*, **127**, 128

- NMR spectroscopy, constant-time HQC experiment for, Shaw *et al.*, **124**, 479
- NMR and X-ray structures, conformational database potential for refinement of, improvements and extensions, Kuszewski, Gronenborn, and Clore, **125**, 171
- oligomeric state in solution, determination from pulsed-field-gradient self-diffusion coefficient measurements, comparison of experimental, theoretical, and hard-sphere approximated values, Krishnan, **124**, 468
- paramagnetic, multiplet splittings in, electron spin–nuclear spin cross-correlation effects on, Ghose and Prestegard, **128**, 138
- side-chain amide protons in, stereospecific assignment with H₂NCO-E.COSY, Löhr and Rüterjans, **124**, 255
- side-chain interactions, applicability of influence of scalar-coupled deuterium on ¹⁵N relaxation as probe, Boyd *et al.*, **124**, 61
- uniformly ¹⁵N/¹³C-labeled, assignment and pH titration of carboxylate groups in, 2D NMR experiments H(C)CO₂ and HCCO₂ for, Pellecchia *et al.*, **124**, 274
- uniformly ¹⁵N-labeled, ¹H T_{1ρ} measurement with heteronuclear 2D spectroscopy, Almeida and Opella, **124**, 509
- Proton chemical-shift anisotropy
- amide, determination in ¹⁵N-labeled proteins using ¹H CSA/¹⁵N–¹H dipolar and ¹⁵N CSA/¹⁵N–¹H dipolar cross-correlation rates, Tessari *et al.*, **127**, 128
 - effect on MAS spectra of hydrate crystals, Tekely, **127**, 238
- Proton chemical-shift correlation
- gradient-enhanced 1D, with full sensitivity, Uhrin and Barlow, **126**, 248
- Pulsed electron-nuclear double resonance
- at large thermal spin polarizations, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- Pulsed electron paramagnetic resonance
- with field cycling and bridged loop–gap resonator made by chemical deposition of silver, Sturm, Lötzer, and Voitländer, **127**, 105
 - species selection in divalent rhodium hexacyanide complex using, Coelho Neto and Vugman, **125**, 242
 - transmission-line resonator for, Koptioug, Reijerse, and Klaassen, **125**, 369
- Pulsed-field gradients
- based 1D and 2D multiplicity-edited HSQC experiments, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
 - based velocimetry methods, strategies for NMR rheometry by, Gibbs *et al.*, **125**, 43
 - B₀ field plotting and shimming without, projection-reconstruction spectroscopic imaging for, Gregory, **129**, 173
 - diffusion experiments, effect of nonconstant magnetic-field gradient, Brownian-dynamics computer simulation study, Håkansson *et al.*, **124**, 343
 - diffusive diffraction in cylindrical pore, Gibbs, **124**, 223
 - double-quantum experiments recorded with only z gradients, reduction of residual H₂O signal, Dalvit and Böhlen, **126**, 149
 - enhanced double-quantum-filtered COSY pure absorption spectra, artifact-free, including gradient pulse in evolution period, Ancian *et al.*, **125**, 348
 - enhanced 1D proton chemical-shift correlation with full sensitivity, Uhrin and Barlow, **126**, 248
 - enhanced 1D and 2D HMQC, optimal detection of weak ¹H–¹¹⁹Sn couplings by, application to tin derivative of erythromycin A, Martins *et al.*, **124**, 218
 - and heteronuclear cross polarization, in doubly sensitivity-enhanced 3D HCCH–TOCSY of ¹³C-labeled in H₂O, Wijmenga, Steensma, and van Mierlo, **124**, 459
 - 1D NOE experiments using, Stott *et al.*, **125**, 302
 - quick recording of pure absorption 2D TOCSY, ROESY, and NOESY spectra using, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
 - self-diffusion coefficient measured using, in determination of protein oligomeric state in solution, comparison of experimental, theoretical, and hard-sphere approximated values, Krishnan, **124**, 468
- Pulsed-field-gradient stimulated echo
- diffusion measurements
 - heterogeneous media, Sørland, Hafskjold, and Herstad, **124**, 172
 - short-time, Sørland, **126**, 146
- Pulsed-gradient spin-echo method
- matrix formalism for spin echo analysis of restricted diffusion under generalized gradient waveforms, Callaghan, **129**, 74
 - NMR measurements of convection in capillary, Manz, Seymour, and Callaghan, **125**, 153
- Pulses
- adiabatic (*see* Adiabatic pulses)
 - amplitude-modulated decoupling, in liquid-state NMR, Geen and Böhlen, **125**, 376
 - arbitrary N, spin echoes after, Kim and Lee, **125**, 114
 - selective adiabatic, optimization, Rosenfeld, Panfil, and Zur, **126**, 221
 - selective adiabatic inversion, design using adiabatic condition, Rosenfeld, Panfil, and Zur, **129**, 115
 - soft, in ²⁷Al quadrupolar central transition NMR studies of ovotransferrin, Aramini, Germann, and Vogel, **129**, 111
 - spin-lock, added to MARF imaging sequence, slow dynamics mapping of large-linewidth solids by, De Luca *et al.*, **126**, 159
- Pulse scheme
- HN(CA)NH, for triple-resonance 4D correlation of sequential amide protons and nitrogens-15 in deuterated proteins, Ikegami *et al.*, **124**, 214
- Pulse sequences
- broadband polarization transfer under MAS, application to total through-space-correlation spectroscopy, Baldus and Meier, **128**, 172
 - CPMG (*see* Carr–Purcell–Meiboom–Gill)
 - for flow evaluation, based on self-refocused RF and interleaved spiral readout, Takahashi, Li, and Stødkilde-jørgensen, **126**, 127
 - kin HEHAHA: heteronuclear Hartmann–Hahn transfer with different bandwidths for spins I and S, Carlomagno, Luy, and Glaser, **126**, 110
 - multiple π, phase-cycling schemes for, comparative studies, Igumenova, Mitchell, and Evans, **127**, 144
 - novel element, for biselective and independent rotations with arbitrary flip angles and phases for I and I{S} spin systems, Briand and Sørensen, **125**, 202
 - spin lock, spin $\frac{7}{2}$ excited by, detection of double- and quadruple-quantum coherences for, Ageev, Mann, and Sanctuary, **128**, 12
 - stripe-COSY and superstripe-COSY, combined with selective deuteration strategy, improved measurement of ¹H–¹H coupling constants via, Yang *et al.*, **129**, 212
 - 3D MAXY-HMQC, Liu *et al.*, **129**, 67
 - Water-PRESS, optimization, and integration into pulse sequences for study of biological macromolecules, Price, Hayamizu, and Arata, **126**, 256
- Pure-phase spectroscopy
- multidimensional, by reference-frequency shift, Venkata Raman and Chandrakumar, **125**, 188
 - pure-phase homo- and heteronuclear J-spectra with tilted cross peaks for determination of coupling constants, Koźmiński *et al.*, **125**, 193
- Q
- Quadrupolar nuclei
- multiple-quantum MAS NMR spectra, indirect spin–spin coupling in, Wu *et al.*, **124**, 237
 - quadrupolar relaxation of spin 3 in intermediate ω₀τ_c regime, Baram and Bendel, **129**, 10
 - and spin- $\frac{1}{2}$ nuclei, high-resolution heteronuclear correlation using multiple-quantum MAS, Wang, De Paul, and Bull, **125**, 364

- T_2 , magnetic field inhomogeneity effect measured by multiple-quantum-filtered NMR, Eliav *et al.*, **128**, 82
- 2D multiple quantum MAS NMR
acquisition of whole echo, Brown and Wimperis, **124**, 279
comparison of methods, Brown and Wimperis, **128**, 42
- Quadrupole couplings
deuterium, solution NMR characterization of hydrogen bonds in protein by indirect measurement of, LiWang and Bax, **127**, 54
magnetic field dependence, Filsinger *et al.*, **125**, 280
residual, and biexponential relaxation, ^{23}Na , in simultaneous acquisition and separation of quadrupolar and double-quantum signals, Jung, Cannon, and Katz, **129**, 130
- Quantum treatment
of intermolecular multiple-quantum coherences with intramolecular J coupling in solution NMR, Ahn, Warren, and Lee, **128**, 114
- Quartz crystal temperature sensor
for MAS NMR, Simon, **128**, 194
- R
- Radial spectroscopic imaging
suitable for plants with cylindrical stem symmetry, Meininger *et al.*, **125**, 325
- Radiation damping
intensity jumping and beating in inversion-recovery experiments of water due to, Chen, Mao, and Ye, **124**, 490
suppression in PFG DQ experiments recorded with only z gradients, Dalvit and Böhlen, **126**, 149
- Radiation dosimetry
by localized magnetic resonance spectroscopy, Roser, **124**, 271
- Radicals
methyl-rotor electron-spin dynamics in Smoluchowski drift-diffusional framework, Sørnes and Benetis, **125**, 52
- Radiofrequency
phases and frequencies in NMR, signs of, Levitt, **126**, 164
- Radiofrequency field
calculation in three dimensions: effects of shield geometry on field strength and homogeneity in birdcage coil, Collins *et al.*, **125**, 233
combination of slow and fast modulation for improved cross polarization in solid-state MAS NMR, Hediger *et al.*, **125**, 291
distribution in cardiac MRI, simulation as function of static magnetic field, Singerman *et al.*, **125**, 72
sample-induced perturbations, in high-field high-resolution NMR spectroscopy, Crozier *et al.*, **126**, 39
self-refocused pulse, and interleaved spiral readout, pulse sequence for flow evaluation based on, Takahashi, Li, and Stødkilde-jørgensen, **126**, 127
transverse, for MRI imaging, solenoid-like coil producing, Jeong *et al.*, **127**, 73
- Radiofrequency field gradients
in excitation sculpting, with application to 2D HSQC, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80
in modification of BIRD/TANGO sequences to eliminate uncoupled magnetization, Sodickson and Cory, **125**, 340
- Radiofrequency pulses
selective adiabatic, optimization, Rosenfeld, Panfil, and Zur, **126**, 221
selective adiabatic inversion, design using adiabatic condition, Rosenfeld, Panfil, and Zur, **129**, 115
- ^{87}Rb
2D multiple quantum MAS NMR, comparison of methods, Brown and Wimperis, **128**, 42
- Real-time response
and phase-sensitive detection, demonstration of validity of ESR–STM results, Manassen, **126**, 133
- REDOR (*see* Rotational-echo double resonance)
- Reference-frequency shift
pure-phase multidimensional spectroscopy by, Venkata Raman and Chandrakumar, **125**, 188
- Refocusing
broadband adiabatic, without phase distortion, Hwang, van Zijl, and Garwood, **124**, 250
- RELAX
program based on complete-relaxation-matrix formalism, back calculation of NOESY spectra with, Görler and Kalbitzer, **124**, 177
- Relaxation
accelerated, of sensitive nucleus, for enhancement of signal-to-noise with time, Homer, Perry, and Palfreyman, **125**, 20
backbone carbonyl carbons in ^{13}C , ^{15}N -labeled protein, mechanisms, Allard and Härd, **126**, 48
biexponential, and residual quadrupolar coupling, ^{23}Na , in simultaneous acquisition and separation of quadrupolar and double-quantum signals, Jung, Cannon, and Katz, **129**, 130
electron–nuclear dipolar, for AsO_4^{3-} spin probe in paraelectric phase of KH_2AsO_4 , ESR study, Rakvin and Merunka, **126**, 87
homonuclear cross-correlation cross-relaxation rates along effective field, application to dipole–dipole cross-correlation, Desvieux, **127**, 1
laser-polarized ^{129}Xe in blood foam, Tseng *et al.*, **126**, 79
 ^{15}N data analysis, applicability of model-free approach, Korzhnev, Orekhov, and Arseniev, **127**, 184
NMR experimental-parameter selection based on, graphical approach, Early, Donahue, and Williams, **125**, 163
 ^{15}N nucleus, effect of scalar-coupled deuterium and use as probe for side-chain interactions in proteins, Boyd *et al.*, **124**, 61
nuclei of spin greater than $\frac{1}{2}$ in presence of, magnetic equivalence, Szymański, **127**, 199
quadrupolar, of spin 3 in intermediate $\omega_0\tau_c$ regime, Baram and Bendel, **129**, 10
spin, induced by chemical shielding anisotropy, evaluation: importance of antisymmetric component, Kowalewski and Werbelow, **128**, 144
spin–lattice
and diffusion, measurements using MR signals from laser-hyperpolarized ^{129}Xe nuclei, Patyal *et al.*, **126**, 58
dynamic measurement using snapshot-FLASH MRI, Jivan *et al.*, **127**, 65
- ^1H
distribution in lung, and wet/dry ratio, Estilaei *et al.*, **124**, 410
relative motion of indole ring of tryptophans in gramicidin analogs incorporated into SDS micelles, Hinton and Washburn-McCain, **125**, 259
 $T_{1\rho}$, measurement in uniformly ^{15}N -labeled protein with heteronuclear 2D spectroscopy, Almeida and Opella, **124**, 509
in human brain at 4.1 T, multislice imaging, application of general approach to error estimation and optimized experiment design, Mason, Chu, and Hetherington, **126**, 18
measurement in STEAM progressive saturation experiment, effect of long echo times, Knight-Scott and Li, **126**, 266
1,3,7,10-tetramethylbenzo[*c*]cinnoline: ^{13}C NMR study of internal rotation of mutually interacting methyl groups, Wimmer and Müller, **129**, 1
 $T_{1\rho}$ filter MARF imaging of large-linewidth solids, De Luca *et al.*, **126**, 159
- spin–spin
apparent, time-domain quantitation by wavelet-transform analysis, Serrai *et al.*, **124**, 20
distributions, lineshapes, and weighting techniques, for characterization of fluid distributions in fractured systems, Chang *et al.*, **126**, 213
fat and water protons, and relative concentrations of protons, single-scan imaging technique for measurement of, Ma *et al.*, **125**, 92

- ¹H
 distribution in lung, and wet/dry ratio, Estilaei *et al.*, **124**, 410
 relative motion of indole ring of tryptophans in gramicidin analogs incorporated into SDS micelles, Hinton and Washburn-McCain, **125**, 259
- ²³Na, and content ratio, measurement in phantoms simulating biological systems by use of multiple-quantum filtering, Jung, Cannon, and Katz, **124**, 393
- quadrupolar nuclei, magnetic field inhomogeneity effect measured by multiple-quantum-filtered NMR, Eliav *et al.*, **128**, 82
- splittings, high-resolution proton spectra without, methods for obtaining: proton chemical-shift spectra, Simova, Sengstschmid, and Freeman, **124**, 104
- systematic errors associated with off-resonance oscillations, removal, Czisch, King, and Ross, **126**, 154
- 2D NOE spectra analysis, uncertainties arising from spectral noise, investigation, Likić and Prendergast, **124**, 200
- Relaxation agents
 noble-gas, Hitchens and Bryant, **124**, 227
- Relaxation rates
¹H longitudinal modes, measurement, Norwood, **125**, 265
 measurement from 2D spectra with partial overlap, Mishra *et al.*, **125**, 358
- Relaxation times
 in proteins, optimal sampling strategies for measurement, Jones, **126**, 283
- REPULSION
 approach to efficient powder averaging in solid-state NMR, Bak and Nielsen, **125**, 132
- Resolution
 enhancement, in out-and-back triple-resonance experiments, applied to HCACO sequence, Baur and Kessler, **126**, 270
 in high-field EPR spectroscopy of undiluted Cr(V) salts, $S = \frac{1}{2}$, relationship to exchange effects and *g*-strain broadening, Cage *et al.*, **124**, 495
 importing into evolution dimension of multidimensional NMR spectrum, McGeorge *et al.*, **129**, 134
- Resonances
 backbone, ¹⁵N(*i*+1), ¹³Ca(*i*), and ¹Ha(*i*), in ¹³C/¹⁵N-labeled proteins, correlation by (CO)N(CO)CAH experiment, Dijkstra *et al.*, **125**, 149
- Resonant frequency
in vivo ESR: longitudinally detected ESR measurements at microwave regions of 300, 700, and 900 MHz in rats treated with nitroxide radical, Yokoyama *et al.*, **129**, 201
- Resonant modes
 birdcage coil, Leifer, **124**, 51
- Resonator
 bird-cage, mutual inductance in, Tropp, **126**, 9
 bridged loop-gap, made by chemical deposition of silver, pulsed EPR with field cycling using, Sturm, Lötzer, and Voitländer, **127**, 105
 double-stacked dielectric, for sensitive EPR measurements, Jaworski, Sienkiewicz, and Scholes, **124**, 87
 shielded-loop, planar quadrature coil design using, Stensgaard, **125**, 84
 transmission-line, for pulsed EPR, Koptioug, Reijerse, and Klaassen, **125**, 369
- Rheometry
 NMR-based, techniques based on MRI velocimetry, Gibbs *et al.*, **125**, 43
- Rhodium hexacyanide complex
 [Rh(CN)₆]⁴⁻
¹³C EPR hyperfine interaction in KCl host lattice, Vugman, Giannoni, and Coelho Neto, **124**, 352
 divalent, species selection using pulsed EPR, Coelho Neto and Vugman, **125**, 242
- Ribose
 ribose-base sequential NOEs, identification according to base types in uniformly ¹³C-labeled RNAs, Ramachandran *et al.*, **124**, 210
- RNA
¹³C-uniformly labeled, base types in, identification of ribose-base sequential NOEs according to, Ramachandran *et al.*, **124**, 210
- ROESY (*see* Rotating-frame Overhauser effect spectroscopy)
- Rotating frame
 tilted, under MAS in solids, selective homonuclear polarization transfer in, Takegoshi, Nomura, and Terao, **127**, 206
- Rotating-frame imaging
 2D NQR, Robert and Pusiol, **127**, 109
- Rotating-frame Overhauser effect spectroscopy
 coherence transfer distortions, origin of correlation time dependence, Ghose, Evans, and Prestegard, **128**, 207
 HOHAHA distortions of spectra, selection of spin-lock transmitter position for minimization, Chan *et al.*, **126**, 183
 method for simulation of spectra, Allard, Helgstrand, and Härd, **129**, 19
 off-resonance
 complete-relaxation-matrix analysis of spectra, for DNA duplex with G-A mismatch in solution, Kuwata *et al.*, **128**, 70
 method for simulation of spectra, Allard, Helgstrand, and Härd, **129**, 19
 and TOCSY and NOESY, pure absorption 2D spectra, quick recording using pulsed field gradients, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
 with water flip back, for high-field NMR of biomolecules, Fulton and Ni, **129**, 93
- Rotational-echo double resonance
 dephasing, by multiple spins in presence of molecular motion, Goetz and Schaefer, **127**, 147
 sidebands, orientational information in solids from, Goetz and Schaefer, **129**, 222
- Rotational resonance
 zero-quantum correlation spectroscopy under conditions of, determination of interatomic distances by, Koons *et al.*, **124**, 499
- Rotations
 biselective and independent, with arbitrary flip angles and phases for I and I{S} spin systems, novel pulse sequence element for, Briand and Sørensen, **125**, 202
 internal, mutually interacting methyl groups, ¹³C NMR study, Wimmer and Müller, **129**, 1
- S
- Sample flipping
 2D dipolar spectra with, determination of orientational anisotropy in glassy solids by, Utz *et al.*, **128**, 217
- Sample length
 variable, line-like samples with, analysis of movement along *x*-axis of double TE₁₀₄ and single TE₁₀₂ rectangular cavity, Mazúr, Morris, and Valko, **129**, 188
- Samples
 induction of RF perturbations in high-field high-resolution NMR spectroscopy, Crozier *et al.*, **126**, 39
 NMR, temperature control, thermoelectric cooling for, Gregory, Claridge, and Leonard, **124**, 228
 programmed translation cycles, fresh spins for NMR signal enhancement using, Wu and Johnson, **127**, 225
- Sampling
 cyclic, fresh spins for NMR signal enhancement using, Wu and Johnson, **127**, 225
 optimal, for measurement of relaxation times in proteins, Jones, **126**, 283
- Sapphire
²⁷Al chemical shielding anisotropy, Vosegaard and Jakobsen, **128**, 135

- Saturation transfer
steady-state, off-resonance irradiation effect, Baguet and Roby, **128**, 149
- Scanning tunneling microscopy
–ESR results, validity, demonstration with real-time response and phase-sensitive detection, Manassen, **126**, 133
- Sciatic nerve
compartments in, discrimination by ^2H double-quantum-filtered NMR, Shinar, Seo, and Navon, **129**, 98
- Second-nearest-neighbor effects
on N NMR shieldings in models for solid Si_3N_4 and C_3N_4 , Tossell, **127**, 49
- Selective excitation
adiabatic slice-selective, for surface coils, Shen and Rothman, **124**, 72
singly and doubly selective 1D experiments using, application of excitation sculpting to construction of, Gradwell, Kogelberg, and Frenkiel, **124**, 267
- Selective homonuclear polarization transfer
in tilted rotating frame under MAS in solids, Takegoshi, Nomura, and Terao, **127**, 206
- Self-consistent-field calculations
and off-angle fast-sample-spinning NMR, for diazo systems: studies of isolated ^{15}N – ^{15}N spin pair, Challoner, Harris, and Tossell, **126**, 1
- Self-diffusion coefficient
pulsed-field-gradient, in determination of protein oligomeric state in solution, comparison of experimental, theoretical, and hard-sphere approximated values, Krishnan, **124**, 468
- Sensitive nuclei
accelerated relaxation for enhancement of signal-to-noise with time, Homer, Perry, and Palfreyman, **125**, 20
- Sensitivity
doubly sensitivity enhanced 3D HCCH–TOCSY of ^{13}C -labeled proteins in H_2O using heteronuclear cross polarization and pulsed-field gradients, Wijmenga, Steensma, and van Mierlo, **124**, 459
fast chemical shift imaging methods, comparison, Pohmann, von Kienlin, and Haase, **129**, 145
full, gradient-enhanced 1D proton chemical-shift correlation with, Uhrin and Barlow, **126**, 248
improvement
in gradient-based 1D and 2D multiplicity-edited HSQC experiments, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
in selective ^1H – ^{13}C 1D polarization-transfer schemes, Parella, Sánchez-Ferrando, and Virgili, **126**, 278
- Separated-local-field experiment
high-resolution 3D, with magic-angle turning, Hu *et al.*, **126**, 120
- Shield geometry
effects on B_1 field strength and homogeneity in birdcage coil, calculation method, Collins *et al.*, **125**, 233
- Shielding
low-frequency magnetic interference in weak-field MRI by single-layer cylindrical coil, Planinšič, **126**, 30
nitrogen (*see* Nitrogen shieldings)
- Shimming
automated
for deuterated solvents, using field profiling, Sukumar *et al.*, **125**, 159
with normal spectrometer hardware, practical method for, Barja *et al.*, **125**, 197
 B_0 field, without pulsed gradients, projection-reconstruction spectroscopic imaging for, Gregory, **129**, 173
high-resolution MAS probe, Sodickson and Cory, **128**, 87
- Shims
on-axis, for high-resolution NMR, fast automatic adjustment, Shen and Rothman, **127**, 229
- Sidebands
in adiabatic decoupling
coherence sidebands, elimination, Bendall and Skinner, **129**, 30
effect of sweep direction, Kupče, **129**, 219
reducing, phase-cycling algorithm for, Skinner and Bendall, **124**, 474
dipolar spinning, in MAS proton spectra of hydrate crystals, effect of proton chemical-shift anisotropy, Tekely, **127**, 238
REDOR, orientational information in solids from, Goetz and Schaefer, **129**, 222
spinning, in slow-MAS NMR spectra arising from tightly J -coupled spin pairs, Wu *et al.*, **124**, 366
- Side chains
interactions in proteins, applicability of influence of scalar-coupled deuterium on ^{15}N relaxation as probe, Boyd *et al.*, **124**, 61
- Signal class recognition
automated, by Bayesian method, use of global symmetries in, Schulte *et al.*, **129**, 165
- Signal enhancement
fresh spins for, through programmed sample translation cycles, Wu and Johnson, **127**, 225
- Signal intensity
jumping and beating due to radiation damping in inversion-recovery experiments of water, Chen, Mao, and Ye, **124**, 490
- Signal-to-noise ratio
enhancement with time, accelerated relaxation of sensitive nucleus for, Homer, Perry, and Palfreyman, **125**, 20
intrinsic, in cardiac MRI
at 1.5, 3, and 4 T, Wen *et al.*, **125**, 65
simulation as function of static magnetic field, Singerman *et al.*, **125**, 72
- Signals
internal and external, in NMR spectra of plant tissues, use of bulk magnetic susceptibility to resolve, Shachar-Hill *et al.*, **127**, 17
noisy, detection–estimation scheme for, applications to delayed acquisition data, Lin *et al.*, **128**, 30
tissue, flow-driven arterial water stimulation with elimination of, Marro, **124**, 240
- Sign determination
absolute sign of hyperfine interaction: pulsed ENDOR spectroscopy at large thermal spin polarizations, Bennebroek and Schmidt, **128**, 199
- Signs
of frequencies and phases in NMR, evaluation, Levitt, **126**, 164
small $J(^1\text{H}, ^{13}\text{C})$ coupling constants in linear spin systems, DQ/ZQ NMR experiment for determination of, Otting, **124**, 503
- Silver
chemical deposition, bridged loop–gap resonator made by, pulsed EPR with field cycling using, Sturm, Lötzer, and Voitländer, **127**, 105
- Simulations
 B_1 field distribution and intrinsic signal-to-noise ratio in cardiac MRI as function of static magnetic field, Singerman *et al.*, **125**, 72
computer
Brownian-dynamics, in study of influence of nonconstant magnetic-field gradient on PFG NMR diffusion experiments, Håkansson *et al.*, **124**, 343
NOESY, ROESY, and off-resonance ROESY spectra, method for, Allard, Helgstrand, and Härd, **129**, 19
EPR behavior of internal motion of methyl fragment in radicals, using Smoluchowski drift diffusion model, Sørnes and Benetis, **125**, 52
- Si_3N_4
solid, N NMR shieldings in models for, second-nearest-neighbor effects, Tossell, **127**, 49
- SLIM (*see* Spectral localization by imaging)
- Smoluchowski model
drift diffusion, methyl-rotor electron-spin dynamics using, Sørnes and Benetis, **125**, 52

- ¹¹⁹Sn
and ¹⁹F, solid organotin fluorides, multinuclear experiments, Cherryman and Harris, **128**, 21
weak ⁿJ(¹H–¹¹⁹Sn) couplings, optimal detection by gradient-enhanced 1D and 2D HMQC, application to erythromycin A derivative Ery(OSn(t-Bu)₂)₂O, Martins *et al.*, **124**, 218
- Snapshot-FLASH (*see* Fast low-angle shot, snapshot)
- Sodalite
⁵⁷Fe-substituted, X-band pulsed ENDOR study: effect of zero-field splitting, Vardi *et al.*, **126**, 229
- Sodium
intracellular, in isolated perfused rat heart in absence of chemical-shift reagent, multiple-quantum-filtered ²³Na NMR in monitoring of, Tauskela *et al.*, **127**, 115
- Sodium borocaptate
¹⁰B, quadrupolar relaxation of spin 3 in intermediate $\omega_0\tau_c$ regime, Baram and Bendel, **129**, 10
- Sodium dodecyl sulfate
micelles, tryptophans in gramicidin analogs incorporated into, relative motion of indole ring, proton *T*₁, *T*₂, and NOE study, Hinton and Washburn-McCain, **125**, 259
- Sodium nitroprusside
¹⁴N, quadrupole coupling constant, magnetic field dependence, Filsinger *et al.*, **125**, 280
- Soft pulses
in ²⁷Al quadrupolar central transition NMR studies of ovotransferrin, Aramini, Germann, and Vogel, **129**, 111
- Solenoid coil
producing transverse RF fields for MR imaging, Jeong *et al.*, **127**, 73
- Solids
biological solid-state NMR, phase-cycling schemes for multiple π -pulse sequences in, Igumenova, Mitchell, and Evans, **127**, 144
dipolar interactions, far-off-resonance averaging, Chang *et al.*, **124**, 165
glassy, orientational anisotropy determination by 2D dipolar spectra with sample flipping, Utz *et al.*, **128**, 217
large-linewidth, slow dynamics mapping by MARF spin-lock filter, De Luca *et al.*, **126**, 159
molecular motion in, ²H double-quantum NMR spectroscopy for study of, Duer and Stourton, **129**, 44
nuclear-spin propagation, cog-wheel model, Brüscheweiler and Ernst, **124**, 122
organotin fluorides, multinuclear experiments on, Cherryman and Harris, **128**, 21
orientational information from REDOR sidebands, Goetz and Schaefer, **129**, 222
para-H₂, theory of multiple NMR spin echoes of HD impurities in, Kisvarsanyi and Sullivan, **127**, 192
peptide–membrane interactions, NMR analyses, preparation of oriented lipid bilayer on ultrathin polymers for, Augé *et al.*, **124**, 455
powder averaging in magnetic resonance, REPULSION approach, Bak and Nielsen, **125**, 132
rigid, assignment of ¹³C NMR spectra by 2D MAS separated-local-field spectroscopy, Pan, **124**, 1
rocket propellants, imaging at 14.1 T, Maas, Merwin, and Cory, **129**, 105
rotating, with several groups of equivalent nuclei, time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
Si₃N₄ and C₃N₄, N NMR shieldings in models for, second-nearest-neighbor effects, Tossell, **127**, 49
spin diffusion and cross-relaxation in, Müller, Zimmermann, and Haeblerlen, **126**, 66
- Solution NMR
characterization of hydrogen bonds in protein by indirect measurement of deuterium quadrupole couplings, LiWang and Bax, **127**, 54
intermolecular multiple-quantum coherences with intramolecular *J* coupling in, quantum treatment, Ahn, Warren, and Lee, **128**, 114
- Solutions
aqueous, DNA duplex with G–A mismatch in, complete-relaxation-matrix analysis of off-resonance ROESY spectra, Kuwata *et al.*, **128**, 70
polymer, convectional flow in capillary, pulsed-gradient spin-echo NMR measurements, Manz, Seymour, and Callaghan, **125**, 153
protein oligomeric state in, determination from pulsed-field-gradient self-diffusion coefficient measurements, comparison of experimental, theoretical, and hard-sphere approximated values, Krishnan, **124**, 468
- Solution-state studies
heteronuclear *J* cross-polarization, application of calculation of coherence-transfer behavior under planar vs isotropic mixing Hamiltonians, Krishnan and Rance, **124**, 205
- Solvent effects
on oxygen-17 chemical shifts in amides: quantitative linear solvation shift relationships, Diez *et al.*, **124**, 8
- Solvent polarity effects
nitrogen NMR shielding of 1,2,4,5-tetrazine, Witanowski *et al.*, **124**, 127
- Solvents
deuterated, automated shimming using field profiling, Sukumar *et al.*, **125**, 159
isotropic and liquid crystalline, ¹³C–{¹H} spectra of 2,2'-difluorobiphenyl in: X part of ABX spin system, Edgar, Emsley, and Furby, **128**, 105
- Solvent suppression
post-acquisition, by singular-value decomposition, Zhu, Smith, and Hua, **124**, 286
- Spatial modulation
dependence of spin-echo signals on, Jones, Morris, and Waterton, **124**, 291
- Spectra
¹H NMR, homonuclear broadband-decoupled, Zangger and Sterk, **124**, 486
- Spectral line analysis
continuous wavelet transform as tool for, and applications, Barache, Antoine, and Dereppe, **128**, 1
- Spectral localization by imaging
diffusion measurement in phantoms and tissues using, Yang *et al.*, **129**, 161
- Spectrometer
normal hardware, practical method for automated shimming with, Barja *et al.*, **125**, 197
- Spin diffusion
and cross correlation, effect on net NOE enhancement in NMR, Madhu and Kumar, **127**, 168
and cross-relaxation, in solid-state NMR, Müller, Zimmermann, and Haeblerlen, **126**, 66
- Spin dynamics
1D NOE experiments using pulsed-field gradients, Stott *et al.*, **125**, 302
- Spin echo analysis
restricted diffusion under generalized gradient waveforms, matrix formalism for, Callaghan, **129**, 74
- Spin echoes
after arbitrary *N* pulses, Kim and Lee, **125**, 114
intersequence stimulated, generation and elimination in double-quantum filtering, mathematical analysis, Jung and Katz, **124**, 232
long echo time effect on *T*₁ measurement in STEAM progressive saturation experiment, Knight-Scott and Li, **126**, 266
multiple NMR, of HD impurities in solid para-H₂, theory, Kisvarsanyi and Sullivan, **127**, 192
nonlinear stimulated (*see* Nonlinear stimulated echoes)
pulsed-gradient (*see* Pulsed-gradient spin-echo method)

- spatial dependence of signals, Jones, Morris, and Waterton, **124**, 291
- whole, acquisition, in 2D multiple quantum MAS NMR, Brown and Wimperis, **124**, 279
- Spin-lock filter
- MARF, slow dynamics mapping of large-linewidth solids by, De Luca *et al.*, **126**, 159
- Spin-lock sequences
- spin $\frac{1}{2}$ excited by, detection of double- and quadruple-quantum coherences for, Ageev, Mann, and Sanctuary, **128**, 12
- transmitter position selection for minimization of HOHAHA distortions of ROESY spectra, Chan *et al.*, **126**, 183
- Spin- $\frac{3}{2}$ nuclei
- developments in multiple-quantum MAS NMR for, Duer and Stourton, **124**, 189
- Spin- $\frac{1}{2}$ nuclei
- and quadrupolar nuclei, high-resolution heteronuclear correlation using multiple-quantum MAS, Wang, De Paul, and Bull, **125**, 364
- Spin pairs
- ^{15}N - ^{15}N , isolated, in 5-methyl-2-diazobenzenesulfonic acid hydrochloride, off-angle fast-sample-spinning NMR and self-consistent-field calculations, Challoner, Harris, and Tossell, **126**, 1
- spin- $\frac{1}{2}$, dipolar-coupled homonuclear, 1D and 2D MAS NMR spectra of, Kundla *et al.*, **129**, 53
- tightly J -coupled, slow-MAS NMR spectra arising from, spinning sidebands in, Wu *et al.*, **124**, 366
- Spin polarizations
- large thermal, pulsed ENDOR spectroscopy at, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- Spin probes
- AsO_4^{4-} as, in paraelectric phase of KH_2AsO_4 , electron-nuclear dipolar relaxation, ESR study, Rakvin and Merunka, **126**, 87
- nitroxide, internal dynamics in glassy polymer matrix detected by, double-modulation ESR study, Rakvin and Vekslí, **125**, 28
- Spin propagation
- in solids, cog-wheel model, Brüschweiler and Ernst, **124**, 122
- Spins
- arbitrary, nucleus of, electron-spin-echo envelope modulation arising from hyperfine coupling to, Ponti, **127**, 87
- fresh, for NMR signal enhancement, through programmed sample translation cycles, Wu and Johnson, **127**, 225
- greater than $\frac{1}{2}$, nuclei with, magnetic equivalence in presence of relaxation, Szymański, **127**, 199
- multiple, in presence of molecular motion, REDOR dephasing by, Goetz and Schaefer, **127**, 147
- $\frac{7}{2}$, excited by spin lock pulse sequences, detection of double- and quadruple-quantum coherences for, Ageev, Mann, and Sanctuary, **128**, 12
- 3, quadrupolar relaxation in intermediate $\omega_0\tau_c$ regime, Baram and Bendel, **129**, 10
- Spin-spin coupling
- compensation for effects during adiabatic pulses, Kupče and Freeman, **127**, 36
- E.COSY-type measurement of J_{HH} coupling constants, application of spin-state-selective excitation, Meissner, Duus, and Sørensen, **128**, 92
- heteronuclear coupling constants, determination from E.COSY-type cross peaks, HMQC- and HSQC-based 2D NMR experiments: HECADE, Koźmiński and Nanz, **124**, 383
- ^1H - ^1H coupling constants, improved measurement in DNA via stripe-COSY and superstripe-COSY pulse sequences combined with selective deuteration strategy, Yang *et al.*, **129**, 212
- indirect, in multiple-quantum MAS NMR spectra of quadrupolar nuclei, Wu *et al.*, **124**, 237
- intramolecular, in solution NMR, intermolecular multiple-quantum coherences with, quantum treatment, Ahn, Warren, and Lee, **128**, 114
- 3J , antamanide, in illustration of derivation of dihedral-angle restraints for polypeptide-structure determination in presence of conformational equilibria, Schmidt, **124**, 310
- $^1J_{\text{CH}}$ splittings, dipolar contributions to, measurement from magnetic-field dependence of J modulation in 2D NMR spectra, Tjandra and Bax, **124**, 512
- $^3J_{\text{HC}}$ coupling constants, determination in antamanide by 2D NMR multiplet simulation for analysis of conformational equilibria, Schmidt, **124**, 298
- long-range heteronuclear, measuring, sensitivity- and gradient-enhanced heteronuclear coupled/decoupled HSQC-TOCSY experiments for, Kövér, Hruby, and Uhrín, **129**, 125
- measurement of degree of coupled isotopic enrichment of different positions in antibiotic peptide, Miller, Egan, and Townsend, **125**, 120
- pure-phase homo- and heteronuclear J -spectra with tilted cross peaks for determination of coupling constants, Koźmiński *et al.*, **125**, 193
- small $J(^1\text{H}, ^{13}\text{C})$ coupling constants in linear spin systems, determination of signs of, DQ/ZQ NMR experiment for, Otting, **124**, 503
- spinning sidebands in slow-MAS NMR spectra arising from tightly J -coupled spin pairs, Wu *et al.*, **124**, 366
- weak $^nJ(^1\text{H}-^{119}\text{Sn})$, optimal detection by gradient-enhanced 1D and 2D HMQC, application to tin derivative of erythromycin A, Martins *et al.*, **124**, 218
- Spin-state-selective excitation
- application for E.COSY-type measurement of J_{HH} coupling constants, Meissner, Duus, and Sørensen, **128**, 92
- Spin systems
- ABX, in isotropic and liquid crystalline phases, general features of X part: ^{13}C - $\{^1\text{H}\}$ spectra of 2,2'-difluorobiphenyl, Edgar, Emsley, and Furby, **128**, 105
- I and I{S}, biselective and independent rotations with arbitrary flip angles and phases for, novel pulse sequence element for, Briand and Sørensen, **125**, 202
- linear, signs of small $J(^1\text{H}, ^{13}\text{C})$ coupling constants in, DQ/ZQ NMR experiment for determination, Otting, **124**, 503
- pairs of spin orders, estimating cross-relaxation rates among, robust method using simultaneous fits to build-up and decay curves, Najfeld *et al.*, **124**, 372
- Spiral magnetic resonance imaging
- fast, with trapezoidal gradients, Duyn and Yang, **128**, 130
- Spiral readout
- interleaved, and self-refocused RF, pulse sequence for flow evaluation based on, Takahashi, Li, and Stødkilde-Jørgensen, **126**, 127
- Splittings
- multiplet, in paramagnetic proteins, electron spin-nuclear spin cross-correlation effects on, Ghose and Prestegard, **128**, 138
- quadrupolar, ^2H double-quantum-filtered spectra with, discrimination between compartments in sciatic nerve by, Shinar, Seo, and Navon, **129**, 98
- spin-spin, high-resolution proton spectra without, methods for obtaining: proton chemical-shift spectra, Simova, Sengstschmid, and Freeman, **124**, 104
- Sso7d protein
- ^{13}C , ^{15}N -labeled, relaxation mechanisms for backbone carbonyl carbons in, Allard and Härd, **126**, 48
- STEAM (*see* Stimulated echo acquisition mode)
- Stenosis
- model, application of pulse sequence for flow evaluation based on self-refocused RF and interleaved spiral readout, Takahashi, Li, and Stødkilde-Jørgensen, **126**, 127
- Stimulated echo acquisition mode
- progressive saturation experiment, T_1 measurement in, effect of long echo times, Knight-Scott and Li, **126**, 266

- Stimulated-echo method (*see also* Pulsed-field-gradient stimulated echo)
 double-STE diffusion experiments, suppression of convection artifacts
 in, Jerschow and Müller, **125**, 372
- Stochastic optimization
 compact MRI magnet design by, Crozier and Doddrell, **127**, 233
- Stripe-COSY
 and superstripe-COSY pulse sequences, combined with selective deuteration strategy, improved measurement of ^1H - ^1H coupling constants via, Yang *et al.*, **129**, 212
- Structures
 NMR calculation, torsion-angle molecular dynamics as tool for, Stein, Rice, and Brünger, **124**, 154
 NMR and X-ray, proteins and nucleic acids, conformational database potential for refinement of, improvements and extensions, Kuszewski, Gronenborn, and Clore, **125**, 171
- Substitution effects
 gramicidin A analogs in micelles, Hinton *et al.*, **124**, 132
- Superstripe-COSY
 and stripe-COSY pulse sequences, combined with selective deuteration strategy, improved measurement of ^1H - ^1H coupling constants via, Yang *et al.*, **129**, 212
- Susceptibility (*see* Magnetic susceptibility)
- Symmetries
 global, use in automated signal class recognition by Bayesian method, Schulte *et al.*, **129**, 165
- T
- TANGO
 and BIRD, RF gradient sequence to eliminate uncoupled magnetization, Sodickson and Cory, **125**, 340
- Temperature
 NMR sample, control, thermoelectric cooling for, Gregory, Claridge, and Leonard, **124**, 228
 room temperature, and normal pressure, mechanically detected magnetic resonance at, Schaff and Veeman, **126**, 200
- Temperature-programmed desorption
 and ESR, studies of adsorption of di-*tert*-butyl nitroxide on Au(111) and NiO(111), evidence for long-range interactions, Katter *et al.*, **126**, 242
- Temperature sensor
 quartz crystal, for MAS NMR, Simon, **128**, 194
- Tensors
 chemical shift (*see* Chemical-shift tensor)
- 1,3,7,10-Tetramethylbenzo[*c*]cinnoline
 internal rotation of mutually interacting methyl groups, ^{13}C NMR study, Wimmer and Müller, **129**, 1
- 1,2,4,5-Tetrazine
 nitrogen NMR shielding, hydrogen bonding and solvent polarity effects, Witanowski *et al.*, **124**, 127
- Thermal spin polarizations
 large, pulsed ENDOR spectroscopy at, and determination of absolute sign of hyperfine interaction, Bennebroek and Schmidt, **128**, 199
- Thermometer
 quartz crystal, for MAS NMR, Simon, **128**, 194
- Thiostrepton
 HOHAHA distortions of ROESY spectra, selection of spin-lock transmitter position for minimization, Chan *et al.*, **126**, 183
- Three-dimensional finite-element analysis
 method for calculation of B_1 fields in three dimensions using, Collins *et al.*, **125**, 233
- 3D MAXY-HMQC (*see* Maximum-quantum correlation HMQC NMR spectroscopy)
- Three-dimensional spectroscopy
 HCCH-TOCSY, doubly sensitivity-enhanced, ^{13}C -labeled proteins in H_2O using heteronuclear cross polarization and pulsed-field gradients, Wijmenga, Steensma, and van Mierlo, **124**, 459
 high-resolution magic-angle turning separated-local-field experiment, Hu *et al.*, **126**, 120
 PFG DQ experiments recorded with only z gradients, reduction of residual H_2O signal, Dalvit and Böhlen, **126**, 149
- Time delay
 constant-time HQQC experiment for protein NMR spectroscopy, Shaw *et al.*, **124**, 479
- Time domain
 amplitude, chemical shift, apparent $T^*_{2\text{c}}$, and phase, quantitation by wavelet-transform analysis, Serrai *et al.*, **124**, 20
 automated analysis of data, use of continuous regularization in, Totz *et al.*, **124**, 400
 2D NMR observation of coupling across ice-water interface, Weglarz and Peemoeller, **124**, 484
- Time-reverse ODESSA (*see* One-dimensional exchange spectroscopy by sideband alternation, time-reverse)
- Tin
 erythromycin A derivative Ery(OSn(tBu) $_2$) $_2\text{O}$, application of optimal detection of weak $^n\text{J}(^1\text{H}-^{119}\text{Sn})$ couplings by gradient-enhanced 1D and 2D HMQC, Martins *et al.*, **124**, 218
- Tissues
 human leg and head, proton decoupling at 4 Tesla, half-volume coil for, Adriany and Gruetter, **125**, 178
 and phantoms, diffusion measurement using SLIM localization, Yang *et al.*, **129**, 161
 plant, internal and external signals in NMR spectra, use of bulk magnetic susceptibility to resolve, Shachar-Hill *et al.*, **127**, 17
 semisolid tissue phantoms, ^{17}O -decoupled proton MR spectroscopy and imaging in, Stolpen, Reddy, and Leigh, **125**, 1
- Tissue signal
 flow-driven arterial water stimulation with elimination of, Marro, **124**, 240
- TOCSY (*see* Total correlation spectroscopy)
- Torrey-Bloch equations
 in NMR study of molecular diffusion, simple solutions, Kenkre, Fukushima, and Sheltraw, **128**, 62
- Torsion angle
 determination in peptides, application of coupling amplification in 2D MAS NMR, Hong *et al.*, **129**, 85
 molecular dynamics, as tool for NMR structure calculation, Stein, Rice, and Brünger, **124**, 154
- Total correlation spectroscopy
 HCCH-TOCSY, doubly sensitivity-enhanced 3D, ^{13}C -labeled proteins in H_2O using heteronuclear cross polarization and pulsed-field gradients, Wijmenga, Steensma, and van Mierlo, **124**, 459
 and HSQC, sensitivity- and gradient-enhanced heteronuclear coupled/decoupled experiments for measuring long-range heteronuclear coupling constants, Kövér, Hruby, and Uhrín, **129**, 125
 1D gradient-enhanced, and 1D ge-NOESY, proton chemical-shift correlation with full sensitivity using, Uhrín and Barlow, **126**, 248
 and ROESY and NOESY, pure absorption 2D spectra, quick recording using pulsed field gradients, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
- Total through-space-correlation spectroscopy
 application of broadband polarization transfer under MAS, Baldus and Meier, **128**, 172
- Transferrin
 ovotransferrin, soft-pulsed ^{27}Al quadrupolar central transition NMR studies, Aramini, Germann, and Vogel, **129**, 111
- Translation cycles
 programmed sample, fresh spins for NMR signal enhancement using, Wu and Johnson, **127**, 225

- Transmitter
spin-lock, selection of position for minimization of HOHAHA distortions of ROESY spectra, Chan *et al.*, **126**, 183
- Triple resonance
four-dimensional correlation of sequential amide protons and nitrogens-15 in deuterated proteins, HN(CA)NH pulse scheme for, Ikegami *et al.*, **124**, 214
- Triple-resonance experiments
out-and-back, resolution enhancement applied to HCACO sequence, Baur and Kessler, **126**, 270
- Tropolone
solid, dynamic hydrogen disorder: single-crystal NMR study of hydroxyl deuterons, Detken *et al.*, **126**, 95
time-reverse ODESSA experiment, Reichert *et al.*, **125**, 245
- Tryptophan
alanine and glycine substitution for, effects on heterogeneity of gramicidin A analogs in micelles, Hinton *et al.*, **124**, 132
in gramicidin analogs in SDS micelles, relative motion of indole ring, proton T_1 , T_2 , and NOE study, Hinton and Washburn-McCain, **125**, 259
- Tumor cells
breast, MCF7, dynamic contrast-enhanced imaging and analysis at high spatial resolution, Furman-Haran, Grobgeld, and Degani, **128**, 161
glioma, multiple- ^{13}C -labeled cell extracts, ultra-high-resolved HSQC spectra, Willker, Flögel, and Leibfritz, **125**, 216
- TurboFLASH
centric phase-encoded sequence, diffusion measurements with, comparison of imaging strategies for, Coremans *et al.*, **124**, 323
- Two-dimensional J spectroscopy
based methods for obtaining proton chemical-shift spectra, Simova, Sengstschmid, and Freeman, **124**, 104
- Two-dimensional spectroscopy
absorption lineshapes in, and effects of slow motions in complex fluids, Saxena and Freed, **124**, 439
automated signal class recognition by Bayesian method, use of global symmetries in, Schulte *et al.*, **129**, 165
dipolar spectra with sample flipping, determination of orientational anisotropy in glassy solids by, Utz *et al.*, **128**, 217
gradient-based multiplicity-edited HSQC experiments, improved sensitivity, Parella, Sánchez-Ferrando, and Virgili, **126**, 274
H(C)CO₂ and HCCO₂, for assignment and pH titration of carboxylate groups in uniformly $^{15}\text{N}/^{13}\text{C}$ -labeled proteins, Pellecchia *et al.*, **124**, 274
 ^1H chemical-shift imaging of human muscle metabolites, Hu, Willcott, and Moore, **126**, 187
heteronuclear, measurement of ^1H $T_{1\rho}$ in uniformly ^{15}N -labeled protein with, Almeida and Opella, **124**, 509
HSQC, application of use of RF gradients in excitation sculpting, Heikkinen, Rahkamaa, and Kilpeläinen, **127**, 80
magnetic-field dependence of J modulation, measurement of dipolar contributions to $^1J_{\text{CH}}$ splittings from, Tjandra and Bax, **124**, 512
MAS, coupling amplification in, and application to torsion angle determination in peptides, Hong *et al.*, **129**, 85
MAS separated-local-field spectroscopy, assignment of ^{13}C NMR spectra of rigid solids by, Pan, **124**, 1
multifrequency Fourier transform ESR: X/Ku-band spectrometer, Borbat, Crepeau, and Freed, **127**, 155
multiple-quantum MAS, quadrupolar nuclei
acquisition of whole echo, Brown and Wimperis, **124**, 279
comparison of methods, Brown and Wimperis, **128**, 42
multiplet simulation, determination of $^3J_{\text{HC}}$ coupling constants in antamanide by, for analysis of conformational equilibria, Schmidt, **124**, 298
NOE-enhanced J -resolved difference spectroscopy for observation of
NOE from regions of spectral overlap, Grode and Mowery, **126**, 142
1D and 2D MAS NMR spectra of dipolar-coupled homonuclear spin- $\frac{1}{2}$ pair, Kundla *et al.*, **129**, 53
peptides on beads, Jelinek *et al.*, **125**, 185
PFG DQ experiments recorded with only z gradients, reduction of residual H₂O signal, Dalvit and Böhlen, **126**, 149
pure absorption TOCSY, ROESY, and NOESY spectra, quick recording using pulsed field gradients, Parella, Sánchez-Ferrando, and Virgili, **125**, 145
rotating-frame NQR imaging, Robert and Pusiol, **127**, 109
spectra with partial overlap, measurement of relaxation rates from, Mishra *et al.*, **125**, 358
time-domain, observation of coupling across ice–water interface, Weglarz and Peemoeller, **124**, 484
- U
- Ubiquitin
 ^{15}N 2D spectra with partial overlap, measurement of relaxation rates from, Mishra *et al.*, **125**, 358
- V
- Valclavam
degree of coupled isotopic enrichment of different positions in, NMR measurement, Miller, Egan, and Townsend, **125**, 120
- Variable angle sample spinning
and isotope dilution and deuterium decoupling, in measurement of interproton nuclear spin dipolar couplings in liquid crystalline samples, Ciampi, De Luca, and Emsley, **129**, 207
- Vectors
internuclear, in DNA duplex with G–A mismatch in solution, rotational correlation times: complete-relaxation-matrix analysis of O-ROESY spectra, Kuwata *et al.*, **128**, 70
- Velocimetry
MRI, based strategies for NMR rheometry, Gibbs *et al.*, **125**, 43
- Vesicles
intermediate-size, high-resolution spectra using MAS NMR, Traikia *et al.*, **125**, 140
- Volume
intracellular, in isolated rat heart, continuous monitoring during normothermic perfusion and ischemia, Askenasy and Navon, **124**, 42
- W
- Water
and fat, protons, relative concentrations and relaxation times, single-scan imaging technique for measurement of, Ma *et al.*, **125**, 92
flip back, ROESY sequence for high-field NMR of biomolecules, Fulton and Ni, **129**, 93
flow-driven arterial water stimulation with elimination of tissue signal, Marro, **124**, 240
–ice interface, coupling across, observation by 2D time domain NMR, Weglarz and Peemoeller, **124**, 484
inversion-recovery experiments, intensity jumping and beating due to radiation damping, Chen, Mao, and Ye, **124**, 490
residual signal in PFG DQ experiments recorded with only z gradients, reduction, Dalvit and Böhlen, **126**, 149
- Water-PRESS
optimization, and integration into pulse sequences for study of biological macromolecules, Price, Hayamizu, and Arata, **126**, 256
- Waveforms
generalized gradient, spin echo analysis of restricted diffusion under, matrix formalism for, Callaghan, **129**, 74

- Wavelet-transform analysis
 time-domain quantitation of amplitude, chemical shift, apparent T^*_2 , and phase by, Serrai *et al.*, **124**, 20
- Wave velocity
 rapid MR measurement, *in vitro* validation, Kraft *et al.*, **126**, 103
- Weak-diffusion theory
 NMR signal in magnetically heterogeneous media, Jensen and Chandra, **126**, 193
- Weak-field magnetic resonance imaging
 low-frequency magnetic interference in, shielding by single-layer cylindrical coil, Planinšič, **126**, 30
- Weight ratios
 wet/dry, and T_1 and T_2 distributions, ^1H NMR measurements in lung, Estilaei *et al.*, **124**, 410
- X
- X band
 pulse-ENDOR study of ^{57}Fe -substituted sodalite: effect of zero-field splitting, Vardi *et al.*, **126**, 229
- ^{129}Xe
 laser-hyperpolarized nuclei, T_1 and diffusion measurements using MR signals from, Patyal *et al.*, **126**, 58
- laser-polarized, NMR in blood foam, Tseng *et al.*, **126**, 79
 as relaxation agent, Hitchens and Bryant, **124**, 227
- X-ray structures
 proteins and nucleic acids, conformational database potential for refinement of, improvements and extensions, Kuszewski, Gronenborn, and Clore, **125**, 171
- Z
- Zero-field splitting
 in X-band pulsed ENDOR study of ^{57}Fe -substituted sodalite, Vardi *et al.*, **126**, 229
- z gradients
 PFG DQ experiments recorded with, reduction of residual H_2O signal, Dalvit and Böhlen, **126**, 149
- Zinc acetate
 ^{13}C -labeled, 1D and 2D MAS NMR spectra of dipolar-coupled homonuclear spin- $\frac{1}{2}$ pair, Kundla *et al.*, **129**, 53
- Zircon
 X-irradiated, unusual center at 10 K, X-band EPR study, Claridge, Sutton, and Tennant, **125**, 107