

Cumulative Subject Index for 1999¹ Volumes 136-141

Α

Absolute-value spectra

ESEEM, dead time-dependent line distortions in, Van Doorslaer, Sierra, and Schweiger, 136, 152

Absorption spectra

obtaining pure absorption 2D J-spectra, Mutzenhardt, Guenneau, and Canet, **141.** 312

Abundant nuclei

cross-polarization dynamics between, analysis based on spin thermodynamics theory: ¹⁹F and ¹H, Ando, Harris, and Reinsberg, 141, 91

ACCORD-HMBC

modification: IMPEACH-MBC, Hadden, Martin, and Krishnamurthy, 140, 274

Accordian spectroscopy

accurate measurements of multiple-bond 13C-1H coupling constants from phase-sensitive 2D INEPT spectra, Ding, 140, 495

Accordion principle

improved performance accordion heteronuclear multiple-bond correlation spectroscopy: IMPEACH-MBC, Hadden, Martin, and Krishnamurthy, 140, 274

N-Acetylaspartate

cerebral concentrations, in vivo quantitation using natural abundance 13C MRS at 1.5 T, Blüml, 136, 219

N-Acetylglycine

¹³C- and ¹⁵N-labeled, 3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, 138, 193

Acquisition schemes

for diffusion tensor imaging using MRI, comparison, Papadakis et al., 137,

Active-coupling-pattern tilting

pure-phase homonuclear J-modulated HMQC with, for determination of homonuclear coupling constants, Koźmiński, 141, 185

Adenine nucleotides

-Co(II), enzyme bound complexes, paramagnetic effects on nuclear relaxation: role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

Adiabatic pulses

asymmetric, for NH selection, Hwang, van Zijl, and Garwood, 138, 173 in MRI, evolution strategy optimization for, Lunati et al., 138, 48 ADP

-Co(II), enzyme bound complexes, paramagnetic effects on nuclear relaxation: role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

Aerogels

in liquid xenon near critical point, Xenon-131 surface sensitive imaging, Pavlovskaya et al., 137, 258

AlB₂ and LiAlO₂, Hartmann–Hahn match conditions for CP/MAS between two half-integer quadrupolar nuclei, Eastman, 139, 98

¹¹B{²⁷A1} high-resolution heteronuclear correlation spectrum for magnesium aluminoborate glass, Chan, 140, 487

¹ Boldface numbers indicate volume; lightface numbers indicate pagination.

¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of ¹³C-²⁷Al dipolar interactions in solids, van Wüllen and Kalwei, 139, 250

Alanine

multiply labeled, REDOR-determined distances from heterospins to clusters of ¹³C labels, Schaefer, **137**, 272

L-Alanylglycylglycine

polycrystalline doubly 13C-labeled, dual processing of 2D exchange data in MAS NMR, Tycko and Berger, 141, 141

AlB₂

¹¹B, Hartmann-Hahn match conditions for CP/MAS between two halfinteger quadrupolar nuclei, Eastman, 139, 98

Algorithm

for NMR spectral normalization, Romano et al., 138, 115

Alternating optimization method

with a priori knowledge, spectral fitting of NMR spectra using, Bi et al., 140, 108

Aluminum acetylacetonate

¹³C-²⁷Al dipolar interactions in, ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of, van Wüllen and Kalwei, 139, 250

Aluminum lactate

¹³C-²⁷Al dipolar interactions in, ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of, van Wüllen and Kalwei, 139, 250

AMARES

adaptation, for parameter estimation for accurate quantification of ¹H spectra, Sundin et al., 139, 189

in time-domain quantification of series of biomedical MR spectroscopy signals, Vanhamme et al., 140, 120

selective correlation to glycine alpha protons in proteins by multiple-quantum spectroscopy, Bazzo, Cicero, and Barbato, 136, 15

Amino acids

backbone and side chain sites, application of 2D and 3D 1H/13C PISEMA experiments, Gu and Opella, 140, 340

Ammonium formate

deuterated, dipolar-coupled 13C-1H spin pairs, heteronuclear double-quantum MAS NMR, Saalwächter et al., 139, 287

Ammonium tartrate

X-irradiated, electron spin echo study, Brustolon, Zoleo, and Lund, 137, 389 Amphotericin B

quantitative measurement of long-range nuclear Overhauser enhancements, Harris et al., 140, 504

Analytical expressions

coherence-transfer functions for general AMX spin system under isotropic mixing, Schedletzky and Glaser, 123A, 174; erratum, 136, 134

Analytical polarization transfer functions

for four coupled spins $\frac{1}{2}$ under isotropic mixing conditions, Luy, Schedletzky, and Glaser, 138, 19

Analytical solutions

exact product operator evolution of weakly coupled spin- $\frac{1}{2}$ $I_m S_n$ systems during arbitrary RF irradiation of I spins, Skinner and Bendall, 141, 271

high-resolution MR, of mouse brain, application to focal cerebral ischemia models, Beckmann, Stirnimann, and Bochelen, 140, 442

Angular variation

EPR spectrum: simulation of polycrystalline EPR spectrum, Misra, 137, 83



Anisotropic motion

nitroxide side-chain dynamics in spin-labeled helix-forming peptide by high-frequency EPR, Bennati *et al.*, **139**, 281

Anisotropic orientation

lactate in skeletal muscle, observed by dipolar coupling in ¹H NMR spectroscopy, Asllani *et al.*, **139**, 213

Anisotropic spin interactions

order matrix analysis of residual dipolar couplings using singular value decomposition, Losonczi et al., 138, 334

Anisotropy

comparison of scalar measures used in MR diffusion tensor imaging, Bahn, 139. 1

invariant and orthonormal scalar measures derived from MR diffusion tensor imaging, Bahn, 141, 68

water diffusion in brain, role of effects of local magnetic susceptibility-induced gradients, *in vivo* evaluation, Clark, Barker, and Tofts, **141**, 52

Apnea

evolution of regional intrapulmonary oxygen partial pressure during, quantification by ³He MRI, Deninger *et al.*, **141**, 207

APT

and SEFT, modifications, and ORSAT: ¹³C signal assignment, Beckmann, Dietrich, and Radeglia, **137**, 132

Aqua-metal complexes

low-symmetry, of electron spin quantum number $S = \frac{5}{2}$, paramagnetic proton nuclear spin relaxation theory for, Strandberg and Westlund, **137**, 333 Aqueous solutions

¹²⁹Xe-¹H cross relaxation in, consequences, Stith *et al.*, **139**, 225

Arginine

guanidine groups, in proteins, correlation to delta protons by multiple quantum spectroscopy, Bazzo, Cicero, and Barbato, 136, 15

Artifacts

ABX strong coupling, suppression in heteronuclear scalar and dipolar correlation spectra, Kövér and Batta, 138, 89

attenuation, associated with large gradient pulses in PGSE NMR diffusion measurements, diagnosing and alleviating, Price *et al.*, **139**, 205

dead time-dependent line distortions in absolute ESEEM spectra, Van Doorslaer, Sierra, and Schweiger, 136, 152

introduced by zero-order phase correction in ¹H NMR, and method of elimination by phase filtering, Wild, **137**, 430

J-coupling crosstalk, in 2D ω_1 -filtered E.COSY spectra, estimation with PFG- ω_1 -filtered TOCSY, Xu, Zhang, and Evans, **138**, 127

in sensitivity-enhanced HSQC, Turner, Connolly, and Stern, **137**, 281

systematic F_1 , in 2D NMR, randomized acquisition for suppression of, Bowyer, Swanson, and Morris, **140**, 513

Assignment (see also Resonance assignment)

computer assisted, ¹³C or ¹⁵N edited 3D-NOESY-HSQC spectra using back-calculated and experimental spectra, Görler *et al.*, **137**, 39

protein spectra, amino acid type-selective triple-resonance experiments: ¹H-¹⁵N correlations, Schubert *et al.*, **141**, 34

proton side-chain, multi-quantum HBHA(CBCACO)NH experiment with partially deuterated samples, Gschwind, Kessler, and Gemmecker, 137, 285

signals in ¹³C spectra, ORSAT and modifications of SEFT and APT, Beckmann, Dietrich, and Radeglia, **137**, 132

Asymmetric design

MRI magnet, using hybrid numerical method, Zhao, Crozier, and Doddrell, 141, 340

Asymmetric pulses

adiabatic, for NH selection, Hwang, van Zijl, and Garwood, 138, 173 ATP-utilizing enzymes

-Co(II)-adenine nucleotide complexes, paramagnetic effects on nuclear relaxation in, role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130 Automated NMR spectra assignment

2D NOESY, crambin, with self-correcting distance geometry-based NOAH/ DIAMOD programs, Xu et al., 136, 76

В

 10 F

borocaptate sodium enriched in, line narrowing of $I = \frac{1}{2}$ spins coupled to quadrupolar nuclei in liquids, Bendel and Baram, **141**, 121

AlB₂, Hartmann–Hahn match conditions for CP/MAS between two halfinteger quadrupolar nuclei, Eastman, 139, 98

¹¹B{²⁷Al} high-resolution heteronuclear correlation spectrum for magnesium aluminoborate glass, Chan, 140, 487

multiple-quantum-filtered NMR, detection of boric acid and borate ion binding to cytochrome c, Taler, Eliav, and Navon, **141**, 228

Backbone

protein, one-bond ¹⁵N-¹H coupling constants in, pulse sequences for measurement, Lerche *et al.*, **140**, 259

sites, of amino acids and peptides, application of 2D and 3D ¹H/¹³C PISEMA experiments, Gu and Opella, **140**, 340

Backbone dynamics

parameters, estimation from NMR relaxation data using Lipari–Szabo model-free approach and Bayesian statistical methods, Andrec, Montelione, and Levy, 139, 408

Back calculation

in computer-assisted assignment of ¹³C or ¹⁵N edited 3D-NOESY-HSQC spectra, Görler *et al.*, **137**, 39

Barstar

superslow backbone protein dynamics study by 1D solid-state MAS exchange NMR spectroscopy, Krushelnitsky et al., 138, 244

Bayesian spectral decomposition

bilinear forms, Ochs et al., 137, 161

Bayesian statistical methods

and Lipari–Szabo formalism, estimation of dynamic parameters from NMR relaxation data using, Andrec, Montelione, and Levy, **139**, 408

Berry's phase

in presence of non-adiabatic environment, with application to magnetic resonance, Gaitan, 139, 152

 B_1 field distribution

mapping with nonideal gradients in high-resolution NMR spectrometer, Jerschow and Bodenhausen, 137, 108

Bias estimation

in heteronuclear relaxation experiments: method for determining B_1 field inhomogeneity, Guenneugues, Berthault, and Desvaux, 136, 118

Bicelles

measurement of one-bond ¹⁵N-¹H coupling constants in protein backbone, pulse sequences for, Lerche *et al.*, **140**, 259

Bilinear forms

Bayesian spectral decomposition, Ochs et al., 137, 161

Bilinear rotation decoupling (see BIRD)

Biofilms

in porous media, selective imaging by NMR relaxation, Hoskins et al., 139, 67

Biofluids

doubly and singly ¹³C-labeled metabolites in, separate quantification by HSQC-filtered *J* spectroscopy, Davison, Jones, and Dixon, **137**, 448 Biological buffer solutions

proteins in, capillary array electrophoretic NMR, He et al., 141, 355 Biological systems

sodium ions in ordered environments in, analysis of ²³Na NMR spectra, Kemp-Harper, Wickstead, and Wimperis, **140**, 351

Bipolar magnetic field gradients

PFGSE method for diffusion measurements in presence of internal gradients, Sørland, Aksnes, and Gjerdåker, 137, 397

BIRD

gradient $BIRD_R$ method for selection of uncoupled magnetization, Heikkinen and Kilpeläinen, 137, 93

Birdcage coils

practical aspects, Doty et al., 138, 144

Bloch equations

near-resonance solution, and application to RF pulse design, Xu and Chan, 138, 225

Bloch-Torrey equation

theory of spin echo in restricted geometries under stepwise gradient pulse sequence, Barzykin, **139**, 342

Blood

¹²⁹Xe in, T_1 and role of oxygenation, Albert *et al.*, **140**, 264

Bone

trabecular, surface charge method for computing induced magnetic field in, evaluation, Hwang and Wehrli, 139, 35

Borate ion

binding to cytochrome c, multiple quantum filtered NMR detection, Taler, Eliav, and Navon, **141**, 228

Boric acid

binding to cytochrome c, multiple quantum filtered NMR detection, Taler, Eliav, and Navon, **141**, 228

Borocaptate sodium

enriched in 10 B, line narrowing of $I=\frac{1}{2}$ spins coupled to quadrupolar nuclei in liquids, Bendel and Baram, **141**, 121

Boundary condition

magnetic resonance imaging measurement of volume magnetic susceptibility using, Wang, Li, and Haselgrove, **140**, 477

Brain

human

functional MR imaging using FLASH, effects of imaging parameters, Preibisch and Haase, 140, 162

metabolite concentrations, *in vivo* quantitation using natural abundance ¹³C MRS at 1.5 T, Blüml, **136**, 219

metabolites in, mapping using double echo-filter metabolite imaging technique, Chen and Hu, 140, 363

short-echo-time ¹H NMR spectroscopy, suppression of macromolecules resonances using multiple inversion recovery, Knight-Scott, **140**, 228 single-shot line scan imaging using stimulated echoes, Finsterbusch and Frahm, **137**, 144

water diffusion measurements, effects of local magnetic susceptibilityinduced gradients in vivo, Clark, Barker, and Tofts, 141, 52

human and monkey, diffusion eigenvalues measured by diffusion tensor MR imaging, linear relationship among, Bahn, 137, 33

mouse, high-resolution MR angiography, application to focal cerebral ischemia models, Beckmann, Stirnimann, and Bochelen, 140, 442

rat

¹⁵N-coupled protons, in vivo detection by ISIS localization and multiplequantum editing, Kanamori and Ross, 139, 240

and phantom, simultaneous lactate editing and observation of other metabolites using stimulated echo-enhanced, Lei and Peeling, **137**, 215

short-echo-time ¹H NMR spectra *in vivo*, quantification of 18 metabolites, Pfeuffer *et al.*, **141**, 104

Broadband decoupling

relaxation effects in spin- $\frac{1}{2}$ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali, 136, 27

Buffer solution

proteins in, capillary array electrophoretic NMR of proteins in, He *et al.*, **141**, 355

С

 ^{13}C

aromatic ¹H-¹³C groups in proteins, optimization of 3D HCCH TROSYtype NMR correlation of, Meissner and Sørensen, **139**, 447

- ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of ¹³C-²⁷Al dipolar interactions in solids, van Wüllen and Kalwei, **139**, 250
- ¹³C- and ¹⁵N-labeled octapeptide, measurement of relaxation rates of N^H and H^a backbone protons, Millet *et al.*, **139**, 434
- 13 C $^{-2}$ D dipolar interactions in solids, comparison of REDOR and θ -REDOR for measuring, Gullion, **139**, 402
- ¹³C-²H distance measurements, applications of deuterium REDOR, Sack et al., 138, 54
- ¹³C-labeled DNA duplex, measurement of longitudinal and transverse cross-correlation for ¹³C-¹H dipolar interactions and ¹³C chemical shift anisotropy, Kojima *et al.*, **136**, 169

¹³C-labeled nucleic acids

 3 J(H3', P_{i+1}) and 3 J(H5'/5", P_i) coupling constants in, determination using CT-HMQC, Hu *et al.*, **139**, 181

and protein complexes, ${}^{3}J_{\mathrm{H3'P}}$ and ${}^{3}J_{\mathrm{C4'P}}$ in, 2D { ${}^{31}\mathrm{P}$ } spin-echo-difference constant-time [${}^{13}\mathrm{C}$, ${}^{1}\mathrm{H}$] HMQC experiment for simultaneous determination, Szyperski *et al.*, **140**, 491

¹³C-labeled retinal, anomalous rotational resonance spectra in MAS NMR, Helmle *et al.*, **140**, 379

¹³C natural abundance S³E and S³CT experiments for measurement of *J*-coupling constants between ¹³C^α or ¹H^α and other protons in protein, Sørensen, Meissner, and Sørensen, 137, 237

¹³C, ¹⁵N

enriched samples of transition metal complexes, measurement of magnitude and sign of heteronuclear coupling constants, Otting, Soler, and Messerle, **137**, 413; *erratum*, **139**, 186

magic-angle turning experiments with TPPM decoupling, resolution enhancement in, McGeorge, Alderman, and Grant, 137, 138

¹³C, ¹⁵N-labeled *N*-acetylglycine, 3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, **138**, 193

¹³C, ¹⁵N-labeled DNA oligonucleotides, thymine resonances in, HCCCH experiment for through-bond correlation of, Sklenář, Masse, and Feigon, 137, 345

¹³C, ¹⁵N-labeled proteins

BEST homonuclear adiabatic decoupling for, Zhang and Gorenstein, 138, 281

¹³C^α-¹H^α couplings in, J^{CH}-modulated 2D (HACACO)NH pulse scheme for quantitative measurement of, Hitchens, McCallum, and Rule, **140**, 281

measurement of ${}^{1}J_{NC'}$ and ${}^{2}J_{H^{NC'}}$ couplings from spin-state-selective 2D correlation spectrum, Permi *et al.*, **140**, 32

selective correlation of amide groups to glycine alpha protons by multiple quantum spectroscopy, Bazzo, Cicero, and Barbato, **136**, 15

¹³C, ¹⁵N-labeled RNA, triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in, Wöhnert *et al.*, **139**, 430

combined reduced 4D ¹³C exchange and ¹H spin diffusion experiment for determining length scale of dynamic heterogeneities, Tracht *et al.*, **140**, 460

CPMAS, methylene-only subspectra using double-quantum filtering sequence, Rossi, Subramanian, and Harbison, 141, 159

deuterated ammonium formate, heteronuclear double-quantum MAS NMR, Saalwächter et al., 139, 287

doubly and singly ¹³C-labeled metabolites, separate quantification by HSQC-filtered *J* spectroscopy, Davison, Jones, and Dixon, **137**, 448

doubly labeled polycrystalline L-alanylglycylglycine, dual processing of 2D exchange data in MAS NMR, Tycko and Berger, 141, 141

edited 3D-NOESY-HSQC spectra, computer-assisted assignment using back-calculated and experimental spectra, Görler *et al.*, **137**, 39

feruloylarabinoxylane, band-selective HSQC and HMBC experiments using excitation sculpting and PFGSE, Gaillet *et al.*, **139**, 454

four-¹³C-spin system, interaction tensors determined from rotational resonance MAS NMR lineshapes of, magnitudes and orientations, Dusold, Maisel, and Sebald, 141, 78

glycerol-d8 in DMSO-d6, relaxation effects in system of spin-½ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali, 136, 27

²H, ¹³C, ¹⁵N-labeled proteins, observation of through-hydrogen-bond ^{2h}J_{HC}, Cordier et al., **140**, 510

helical polypeptide labeled with, numerical simulations of MQ NMR signal amplitudes and experimental MQ excitation spectra, Tycko, 139, 302

Hsc-70 SBD, high-resolution 4D HMQC-NOESY-HSQC spectroscopy, Morshauser and Zuiderweg, 139, 232

indirect imaging, mixing sequences for selective heteronuclear *J* cross polarization for: PRAWN, Chandrakumar and Kimmich, **137**, 100

lineshapes, in ¹³CD₂ spin grouping, cross-related quadrupolar spin relaxation and, Werbelow *et al.*, **140**, 1

magic-angle spinning NMR

with composite pulses, Leppert, Heise, and Ramachandran, **139**, 382 using lanthanide ions, probing membrane surfaces and location of membrane-embedded peptides using, Gröbner, Glaubitz, and Watts, **141**, 335

multiple-bond ¹³C-¹H coupling constants, accurate measurements from phase-sensitive 2D INEPT spectra, Ding, **140**, 495

multiple-frequency resonance structure, high-field DNP and ENDOR with, Weis et al., 140, 293

natural abundance ¹³C MRS at 1.5 T, *in vivo* quantitation of cerebral metabolite concentrations using, Blüml, **136**, 219

NMR spectra of liquid crystals with proton homonuclear dipolar decoupling methods, Fung, Ermolaev, and Yu, 138, 28

polyglycine, CP/MAS, Krushelnitsky et al., 138, 244

REDOR-determined distances from heterospins to clusters of ¹³C labels, Schaefer, **137**, 272

selective and extensive labeling, and 2D solid-state NMR, in determination of multiple ϕ -torsion angles in proteins, Hong, **139**, 389

sensitivity-enhanced sim-CT HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH triple-resonance experiments, Swapna and Montelione, 137, 437

signal assignment: ORSAT and modifications of SEFT and APT, Beckmann, Dietrich, and Radeglia, 137, 132

solid-state NMR

distance measurements in proteins, practical methods: constant-time rotational resonance, Balazs and Thompson, 139, 371

selective polarization and spin diffusion in lipid bilayer-bound polypeptide by, Tian, Fu, and Cross, **139**, 377

trehalose, CSA/DD cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

two- and three-dimensional 1 H/ 13 C PISEMA experiments and application to backbone and side chain sites of amino acids and peptides, Gu and Opella, **140**, 340

ubiquitin, solid-state dipolar INADEQUATE NMR spectra with large double-quantum spectral width, Hong, 136, 86

in *p*-xylene/Dianin's inclusion compound, nuclear distance measurements by 2D-RFDR, Zaborowski, Zimmermann, and Vega, **136**, 47

yeast triose-phosphate isomerase, TROSY gradient-enhanced triple-resonance NMR spectroscopy, Loria, Rance, and Palmer, **141**, 180

or ¹H^α and other protons in protein, measurement of *J*-coupling constants between, ¹³C natural abundance S³E and S³CT experiments for, Sørensen, Meissner, and Sørensen, 137, 237

Calcium carbonate

formation, changes in ionic concentrations during, monitoring with MR current density imaging, Beravs, Demšar, and Demsar, 137, 253

Canavan disease

in vivo quantitation of cerebral metabolite concentrations using natural abundance ¹³C MRS at 1.5 T, Blüml, 136, 219 Capillary array electrophoretic NMR

proteins in biological buffer solutions, He et al., 141, 355

Cardiac function

functional MRI, displacement encoding with stimulated echoes in: DENSE, Aletras et al., 137, 247

high-resolution strain analysis with fast-DENSE, Aletras, Balaban, and Wen, 140, 41

Cartilage

bovine nasal, ²³Na NMR spectra, Kemp-Harper, Wickstead, and Wimperis, 140, 351

human articular, *in vivo* triple-quantum-filtered twisted projection sodium MRI, Borthakur *et al.*, **141**, 286

 $^{13}CD_2$

spin grouping, carbon-13 lineshapes in, cross-related quadrupolar spin relaxation and, Werbelow *et al.*, **140**, 1

111**C**d

high-resolution magnetic relaxation dispersion measurements using dualmagnet system, Wagner et al., 140, 172

Cell samples

NMR spectral normalization, algorithm for, Romano et al., 138, 115

Centric k-space sampling

and prepared magnetization, SPRITE MRI with, Mastikhin $\it et~al.,~136,~159~CH_3$

small tunneling splitting: spectroscopy from proton spin magnetization in rotating frame, Damyanovich, Peternelj, and Pintar, **140**, 9

Chaperone

Hsc-70 SBD, high-resolution 4D HMQC-NOESY-HSQC spectroscopy, Morshauser and Zuiderweg, 139, 232

Chelates

lanthanide, as bilayer alignment tools in NMR studies of membrane-associated peptides, Prosser et al., 141, 256

Chemical exchange

intermolecular, detection through decorrelation of two-spin order, Skrynnikov and Ernst, 137, 276

slow, in NMR, selective injection of magnetization by, Boulat, Epstein, and Rance, 138, 268

Chemical exchange relay

editing of exchange relayed NOEs in NMR experiments for observation of protein-water interactions, Melacini, Kaptein, and Boelens, 136, 214

Chemical processes

magnetic resonance current density imaging, Beravs, Demšar, and Demsar, ${\bf 137}, 253$

Chemical-shift anisotropy

¹³C, and ¹³C-¹H dipolar interactions, measurement of longitudinal and transverse cross-correlation between, Kojima *et al.*, **136**, 169

and dipole–dipole interactions, cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

Chemical-shift imaging

beyond k-space: spectral localization using higher-order gradients, Pohmann, Rommel, and von Kienlin, 141, 197

human head and calf muscle, ³¹P CSI study: spectral decomposition using bilinear Bayesian approach, Ochs *et al.*, **137**, 161

mapping brain metabolites using double echo-filter metabolite imaging technique, Chen and Hu, **140**, 363

Chemical shifts

efficient refocusing of one-spin and two-spin interactions for NMR quantum computation, Jones and Knill, 141, 322

Chemical-shift tensors

characterized by 2D multiple-quantum NMR spectroscopy, Medek and Frydman, 138, 298

¹⁵N, of [1-¹⁵N]-2'-deoxyguanosine, magnitudes and orientations determined from polycrystalline sample by 2D solid-state NMR, Lorigan *et al.*, 140, 315 Chloroform

improved liquid-state CSA data, Batta, Kövér, and Kowalewski, 136, 37 Cholesteryl acetate

¹³C signals, assignment: ORSAT and modifications of SEFT and APT, Beckmann, Dietrich, and Radeglia, 137, 132

Chromium(V) complexes

in glassy solution, spin-echo dephasing for, solvent and temperature dependence, Eaton and Eaton, 136, 63

35C1

NaClO₃ polycrystalline sample, reconstructing powder NQR images with real gradient coils, Swaminathan and Suits, **138**, 123

Clay suspensions

⁷Li double-quantum filtered NMR and multinuclear relaxation rates, Grandjean and Robert, 138, 43

⁵⁹Co

salts, shift tensors characterized by 2D multiple-quantum NMR spectroscopy, Medek and Frydman, 138, 298

Coatings

planar, profiling, high-gradient permanent magnet for, Glover et al., 139, 90 Cobalt(II)

-ADP, enzyme bound complexes, paramagnetic effects on nuclear relaxation: role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

Coherence

features, in NMR *q*-space plots, assignment to particular diffusion modes in erythrocyte suspensions, Torres *et al.*, **138**, 135

Coherence pathway selection

by gradients in dipolar coupled solids, Maas et al., 141, 29

stimulated anti-echo selection in spatially localized NMR spectroscopy, Zhu and Smith, 136, 1

Coherence selection

gradient, spectral simulations incorporating, Young et al., 140, 146

Coherence sidebands

methods for characterizing a decoupler channel using undetectable quantum coherences, Bendall and Skinner, 139, 175

Coherence transfer (see also Spin-state-selective coherence transfer)

dipolar coupling-mediated, in homonuclear two spin- $\frac{1}{2}$ solid-state system, Taylor and Ramamoorthy, 141, 18

and Lie algebra, in separation of $^2\mathrm{H}$ MAS NMR spectra by 2D spectroscopy, Kristensen *et al.*, **139**, 314

Coherence-transfer functions

acquisition in real time, single-shot experiments for, Luy and Glaser, 138, 187

for general AMX spin system under isotropic mixing, analytical expressions for, Schedletzky and Glaser, 123A, 174; erratum, 136, 134

Coherence-transfer pathways

selection in high-resolution NMR by pulsed-field gradients design of gradient pulse sequences, Thomas *et al.*, **137**, 10 geometrical analysis, Mitschang, **137**, 1

Coherent averaging-assisted solid state imaging (CASSI)

spin coherence relaxation in rotating frame as microscopy parameter for strongly coupled spin systems, De Luca *et al.*, **139**, 126

Coherent averaging theory

revised analysis: off-resonance multiple-pulse dynamics in solid-state NMR, Cho, **141**, 164

Coils

birdcage, practical aspects, Doty et al., 138, 144

error-tolerant RF Litz coils for NMR/MRI, Doty, Entzminger, and Hauck, 140, 17

high-performance RF, integrated head immobilization system for fMRI at 1.5 T with, Thulborn and Shen, 139, 26

Composite pulses

echo-planar imaging of porous media with spatial resolution below 100 μ m, Manz, Chow, and Gladden, 136, 226

magic-angle spinning NMR spectroscopy with, Leppert, Heise, and Ramachandran, 139, 382

COMPUTE

L-COMPUTE algorithm for simulations of rotational resonance spectra in MAS NMR, Helmle *et al.*, **140**, 379

γ-COMPUTE

efficient spectral simulations in NMR of rotating solids, Hohwy et al., 136, 6

Computer assisted assignment

¹³C or ¹⁵N edited 3D-NOESY-HSQC spectra, using back-calculated and experimental spectra, Görler et al., 137, 39

Computing

EPR powder spectra, using numerical diagonalization of spin Hamiltonian, Morin and Bonnin, 136, 176

Configuration interaction

and Stone's perturbation theory, g-matrix based on, Li et al., 138, 74 Constant-time variable delay

in IMPEACH-MBC, Hadden, Martin, and Krishnamurthy, 140, 274 Continuous flow

gas flow MRI using circulating laser-polarized ¹²⁹Xe, Brunner *et al.*, **138**, 155

Continuous Gaussian exchange model

slow site exchange processes in solution NMR, Schurr et al., 140, 404 Contrast

T*-weighted, magnetic susceptibility artifacts in, microimaging at 14 T using GESEPI for removal of, Yang et al., 141, 1

Contrast-to-noise ratio

functional MR imaging of human brain using FLASH, effects of imaging parameters, Preibisch and Haase, **140**, 162

Convection

and temperature profiles, measurement in liquid samples, Loening and Keeler, 139, 334

Corrections and additions, 138, 191

Correlation

through-bond, thymine resonances in ¹³C-labeled DNA oligonucleotides, HCCCH experiment for, Sklenář, Masse, and Feigon, **137**, 345

Correlation spectroscopy

determination of coupling constants by deconvolution of multiplets in NMR, Jeannerat and Bodenhausen, 141, 133

measurement of ${}^{1}J_{\rm NC'}$ and ${}^{2}J_{\rm HNC'}$ couplings from spin-state-selective 2D correlation spectrum, Permi *et al.*, **140**, 32

multidimensional solid-state NMR, experimental aspects, Ramamoorthy, Wu, and Opella, **140**, 131

Coupled spins

four spins $\frac{1}{2}$ under isotropic mixing conditions, analytical polarization transfer functions for, Luy, Schedletzky, and Glaser, 138, 19

Coupling constants (see J-coupling)

CP-MAS (see Cross polarization-magic-angle spinning)

CPMG

¹H, ¹H-¹⁵N correlated experiments, transverse cross relaxation in, Ishima, Louis, and Torchia, 137, 289

multipulse solid-state NMR, on static and oriented systems, structural parameters from ¹⁹F homonuclear dipolar couplings by, Grage and Ulrich, **138**, 98

Crambin

automated 2D NOESY assignment and structure calculation with self-correcting distance geometry-based NOAH/DIAMOD programs, Xu *et al.*, **136**, 76

Creatine

resonances, in ¹H MR spectra of human skeletal muscle, effect of exercise, Kreis *et al.*, **137**, 350

Cross-correlated relaxation

CSA/DD, comparison of 1D and 2D (unbiased) experimental methods for measuring, Batta, Kövér, and Kowalewski, **136**, 37

Cross-correlation

longitudinal and transverse, between ¹³C-¹H dipolar interaction and ¹³C chemical shift anisotropy, measurement, Kojima *et al.*, **136**, 169

in quadrupolar spin relaxation, and carbon-13 lineshapes in ¹³CD₂ spin grouping, Werbelow *et al.*, **140**, 1

Cross-peak multiplets

in NMR, deconvolution, determination of coupling constants by, Jeannerat and Bodenhausen, 141, 133

Cross polarization

3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, **138**, 193

high-resolution heteronuclear correlation spectrum for quadrupolar nuclei, Chan, 140, 487

selective heteronuclear

J cross polarization, mixing sequences for: PRAWN, Chandrakumar and Kimmich, 137, 100

selective excitation of proton signals in NMR of isotopically labeled macromolecules, Pelupessy, Chiarparin, and Bodenhausen, **138**, 178 Cross-polarization dynamics

between abundant nuclei ¹⁹F and ¹H, analysis based on spin thermodynamics theory, Ando, Harris, and Reinsberg, **141**, 91

Cross polarization-magic-angle spinning

¹³C, methylene-only subspectra using double-quantum filtering sequence, Rossi, Subramanian, and Harbison, **141**, 159

cross-polarization dynamics between ¹⁹F and ¹H, analysis based on spin thermodynamics theory, Ando, Harris, and Reinsberg, **141**, 91

between two half-integer quadrupolar nuclei, Hartmann-Hahn match conditions for, examples, Eastman, 139, 98

Cross relaxation

attenuation of cross-peak intensities in QUIET-BIRD-NOESY, Cutting and Bodenhausen, **140**, 289

in off-resonance ROESY, tilt angle dependence, Cutting, Ghose, and Bodenhausen, 138, 326

¹²⁹Xe-¹H, in aqueous solutions, consequences, Stith et al., **139**, 225

Cross-relaxation rate constant

between two spins, comparison of measurement schemes, Boulat, 139, 354 Cross-relaxation rates

longitudinal and transverse, quantitative measurement, Malliavin *et al.*, **140**, 189

Crosstalk J-coupling correction

in 2D ω_1 -filtered E.COSY spectra, with PFG- ω_1 -filtered TOCSY, Xu, Zhang, and Evans, 138, 127

Cryogenic temperatures

cryogenically coolable microwave limiter, Rinard, Quine, and Eaton, 136, 207

Current density imaging

chemical processes and reactions, Beravs, Demšar, and Demsar, 137, 253 Cytochrome \boldsymbol{c}

boric acid and borate ion binding to, multiple quantum filtered NMR detection, Taler, Eliav, and Navon, **141**, 228

Cytoskeletor

depletion, RBC membranes with, competition between Na⁺ and Li⁺: ²³Na MQF and ⁷Li relaxation study, Srinivasan *et al.*, **140**, 206

D

DANTE

suppression of radiation damping in high-resolution NMR, Barjat, Mattiello, and Freeman, 136, 114

Data acquisition

high-speed system, for RF time-domain EPR spectroscopy/imaging, Subramanian et al., 137, 379

Data processing

inversion of NMR log data sets with different measurement errors, Dunn and LaTorraca, ${\bf 140,\,153}$

measurement of rotating frame and longitudinal relaxation times through fully *J*-decoupled homonuclear spectra, Guenneau *et al.*, **140**, 250

Data quantification

¹H spectra: finite impulse response filter design for solvent suppression and parameter estimation, Sundin *et al.*, **139**, 189 time-domain, of series of biomedical MR spectroscopy signals, Vanhamme

et al., **140,** 120

Data transformation

transforming NMR data despite missing points, Kuethe et al., 139, 18 Dead time-dependent artifacts

line distortions, in absolute ESEEM spectra, Van Doorslaer, Sierra, and Schweiger, 136, 152

Decomposition

spectral, method using bilinear Bayesian approach, Ochs et al., 137, 161 Deconvolution

of multiplets, in NMR, determination of coupling constants by, Jeannerat and Bodenhausen, **141**, 133

reference, in frequency domain, Goez and Heun, 136, 69

SPORT-NMR software for determination of relaxation times in unresolved NMR spectra, Geppi and Forte, **137**, 177

Decorrelation

two-spin order, detection of intermolecular chemical exchange through, Skrynnikov and Ernst, 137, 276

Decoupled spectra

fully J-decoupled homonuclear

measurement of rotating frame and longitudinal relaxation times through, Guenneau et al., 140, 250

quantitative: obtaining pure absorption 2D *J*-spectra, Mutzenhardt, Guenneau, and Canet, **141**, 312

Decoupler calibration

methods for characterizing decoupler channel using undetectable quantum coherences, Bendall and Skinner, 139, 175

Decoupling

BEST homonuclear adiabatic, for ¹³C- and ¹⁵N-double-labeled proteins, Zhang and Gorenstein, **138**, 281

broadband decoupling schemes, evaluation: relaxation effects in spin- $\frac{1}{2}$ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali, 136, 27

effects of weak decoupling fields on line narrowing of $I=\frac{1}{2}$ spins coupled to quadrupolar nuclei in liquids, Bendel and Baram, **141**, 121

multiple-pulse homonuclear, ¹⁹F solid-state NMR magic-angle-turning experiments with, Hughes, Brouwer, and Harris, **138**, 256

proton homonuclear dipolar, in $^{\rm 13}C$ NMR of liquid crystals, Fung, Ermolaev, and Yu, ${\bf 138},\,{\bf 28}$

two-pulse phase-modulation, ¹³C and ¹⁵N magic-angle turning with, resolution enhancement in, McGeorge, Alderman, and Grant, **137**, 138

DENSE

displacement encoding with stimulated echoes, in cardiac functional MRI, Aletras et al., 137, 247

fast-DENSE high-resolution strain analysis of human heart, Aletras, Balaban, and Wen, 140, 41

Density matrix

analysis of *J* coupling-induced fat suppression in DIET imaging, Stables *et al.*, **136**, 143

simulations of effects of J coupling in spin-echo and fast spin-echo imaging, Stables *et al.*, **140**, 305

[1-15N]-2'-Deoxyguanosine

¹⁵N chemical shift, magnitudes and orientations determined from polycrystalline sample by 2D solid-state NMR, Lorigan et al., 140, 315

Detection

electromagnetic and micromechanical, simultaneous, in EPR, Alzetta *et al.*, **141**, 148

parallel: NMR probe for simultaneous acquisition of multiple samples, Fisher et al., 138, 160

Deuteration

partial, enhanced sensitivity with, multi-quantum HBHA(CBCACO)NH experiment for, Gschwind, Kessler, and Gemmecker, 137, 285

Deuterium

 13 C $^{-2}$ D dipolar interactions in solids, comparison of REDOR and θ -REDOR for measuring, Gullion, **139**, 402

REDOR, principles and applications for distance measurements, Sack *et al.*, **138**, 54

Deuterium NMR

membrane peptides, lanthanide chelates as bilayer alignment tools in, Prosser et al., 141, 256

Diagonal peak suppression

in TROSY-type ¹H NMR NOESY spectra of ¹⁵N-labeled proteins, Meissner and Sørensen, **140**, 499

DIAMOD

self-correcting distance gemometry-based program, automated 2D NOESY assignment and structure calculation of crambin with, Xu *et al.*, **136**, 76 Dianin's inclusion compound

-p-xylene, ¹³C distance measurements by 2D-RFDR, Zaborowski, Zimmermann, and Vega, 136, 47

Dielectric resonator

flow and stopped-flow EPR with rapid field scanning based on, Sienkiewicz et al., 136, 137

DIET (Dual interval echo train)

imaging, *J* coupling-induced fat suppression in, Stables *et al.*, **136**, 143 Diffusion

assignment of coherence features in NMR *q*-space plots to particular diffusion modes in erythrocyte suspensions, Torres *et al.*, **138**, 135

brain, eigenvalues measured by diffusion tensor MR imaging, linear relationship among, Bahn, 137, 33

conditions for exponential time-cubed echo delays, Pfitsch, McDowell, and Conradi, 139, 364

measurements in presence of internal gradients, PFGSE method for, Sørland, Aksnes, and Gjerdåker, 137, 397

MRI edge enhancement as diffusive discord of spin phase structure, Stepišnik *et al.*, **137**, 154

PGSE NMR, artifactual attenuation associated with large gradient pulses, diagnosing and alleviating, Price et al., 139, 205

restricted (see Restricted diffusion)

single-shot measurement in laser-polarized gas, Peled *et al.*, **140**, 320 thermally polarized ³He gas in rat lung, Kober *et al.*, **138**, 308 water

invariant and orthonormal scalar measures derived from MR diffusion tensor imaging, Bahn, **141**, 68

measurements in brain, effects of local magnetic susceptibility-induced gradients in vivo, Clark, Barker, and Tofts, 141, 52

Diffusion map

by radiofrequency field gradient NMR microscopy, Valtier, Humbert, and Canet, ${\bf 141},\,7$

Diffusion tensor imaging

linear relationship among brain diffusion eigenvalues measured by, Bahn, 137, 33

magnetic resonance

comparison of acquisition schemes for, Papadakis *et al.*, **137**, 67 comparison of scalar measures used in, Bahn, **139**, 1

invariant and orthonormal scalar measures derived from, Bahn, **141**, 68 Diffusion-weighted imaging

isotropic weighting, optimized pulse sequence for, Cercignani and Horsfield, ${\bf 140,\,58}$

Dihydrofolate reductase

selective injection of magnetization by slow chemical exchange in NMR, Boulat, Epstein, and Rance, 138, 268

Dipolar clusters

spin counting with fast MAS, Geen et al., 138, 167

Dipolar coupling (see also Residual dipolar coupling)

anisotropic orientation of lactate observed by, in ¹H NMR spectroscopy, Asllani *et al.*, **139**, 213

coherence pathway selection by gradients in dipolar coupled solids, Maas et al., 141, 29

¹⁹F homonuclear, structural parameters by multipulse solid-state NMR on static and oriented systems, Grage and Ulrich, 138, 98

HN(α/β -COCA-J) experiment for measurement of ${}^{1}J_{C'C\alpha}$ couplings from 2D [15 N, 1 H] correlation spectrum, Permi *et al.*, **141**, 44

homonuclear, modifications for measurement: solid-state NMR distance measurements on proteins, Balazs and Thompson, 139, 371

2D and 3D ¹H/¹³C PISEMA experiments, Gu and Opella, **140**, 340

Dipolar coupling-mediated coherence transfer

in homonuclear two spin-½ solid-state system, Taylor and Ramamoorthy, 141, 18

Dipolar decoupling

proton homonuclear, in $^{13}\mathrm{C}$ NMR of liquid crystals, Fung, Ermolaev, and Yu, 138, 28

Dipolar-encoded longitudinal magnetization filter

for ¹H NMR imaging of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, **140**, 432

Dipolar field

and multiple spin echoes and multiple quantum coherence: significance of higher-order terms in equilibrium density matrix, Minot, Callaghan, and Kaplan, 140, 200

Dipolar interactions

¹³C-²⁷Al, in solids, ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of, van Wüllen and Kalwei, **139**, 250

 $^{13}\text{C}{^-2}\text{D}$, in solids, comparison of REDOR and θ -REDOR for measuring, Gullion, **139**, 402

¹³C-¹H, and ¹³C chemical shift anisotropy, measurement of longitudinal and transverse cross-correlation between, Kojima *et al.*, **136**, 169

and scalar interactions, role in paramagnetic effects on nuclear relaxation in enzyme-bound Co(II)-adenine nucleotide complexes, Ray, Jarori, and Nageswara Rao, 136, 130

water molecules in tendon, ¹H and ²H homonuclear and heteronuclear MQF NMR, Eliav and Navon, **137**, 295

Dipolar recoupling

experiments in solid-state NMR, accuracy of distance measurements in, Hodgkinson and Emsley, 139, 46

solid-state dipolar INADEQUATE NMR spectra with large double-quantum spectral width, Hong, 136, 86

Dipole-dipole interactions

and chemical-shift anisotropy, cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

Displacement encoding

with stimulated echoes, in cardiac functional MRI: DENSE, Aletras *et al.*, **137**, 247

Distance geometry

self-correcting, NOAH/DIAMOD programs based on, automated 2D NOESY assignment and structure calculation of crambin with, Xu *et al.*, **136**, 76

Distance measurements

applications of deuterium REDOR, Sack et al., 138, 54

¹³C nuclei in p-xylene/Dianin's inclusion compound, by 2D-RFDR, Zaborowski, Zimmermann, and Vega, 136, 47

REDOR-determined, from heterospins to clusters of ¹³C labels, Schaefer, **137**, 272

in solid-state NMR

accuracy, Hodgkinson and Emsley, 139, 46

on large biomolecules, practical methods: constant-time rotational resonance, Balazs and Thompson, 139, 371

DNA

 13 C-labeled, $^{3}J(H3'_{i}, P_{i+1})$ and $^{3}J(H5'_{i}/5''_{i}, P_{i})$ coupling constants in, determination using CT-HMQC, Hu et al., 139, 181

[1-15N]-2'-deoxyguanosine, magnitudes and orientations of 15N chemical shift determined from polycrystalline sample by 2D solid-state NMR, Lorigan et al., 140, 315

duplex, 13C-labeled, measurement of longitudinal and transverse crosscorrelation for ¹³C-¹H dipolar interactions and ¹³C chemical shift anisotropy, Kojima et al., 136, 169

DNA oligonucleotides

¹³C-labeled, thymine resonances in, HCCCH experiment for through-bond correlation of, Sklenář, Masse, and Feigon, 137, 345

DNA-protein complexes

with 13 C-labeled nucleic acids, $^{3}J_{\text{H3'P}}$ and $^{3}J_{\text{C4'P}}$ in, 2D $\{^{31}\text{P}\}$ spin-echodifference constant-time [13C, 1H] HMQC experiment for simultaneous determination, Szyperski et al., 140, 491

Double echo-filter metabolite imaging technique

mapping brain metabolites using, Chen and Hu, 140, 363

Double-quantum cross polarization

methylene-only subspectra in 13C CPMAS, Rossi, Subramanian, and Harbison, 141, 159

Double-quantum dimension

solid-state dipolar INADEQUATE NMR spectra with large double-quantum spectral width, Hong, 136, 86

Double-quantum filter

sequence, methylene-only subspectra in 13C CP MAS using, Rossi, Subramanian, and Harbison, 141, 159

stimulated echo-enhanced, simultaneous lactate editing and observation of other metabolites using, Lei and Peeling, 137, 215

Double-quantum filtered NMR

¹H, imaging of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, 140, 432

⁷Li, of clay suspensions, Grandjean and Robert, **138**, 43

Double-quantum spectroscopy

heteronuclear DQ MAS NMR in dipolar solids, Saalwächter et al., 139, 287 Double-quantum/zero-quantum experiments

measurement of magnitude and sign of heteronuclear coupling constants in transition metal complexes, Otting, Soler, and Messerle, 137, 413; erratum, 139, 186

Dual interval echo train (DIET)

imaging, J coupling-induced fat suppression in, Stables et al., 136, 143 Dual-magnet system

high-resolution magnetic relaxation dispersion measurements of solute spin probes using, Wagner et al., 140, 172

Dynamic heterogeneities

determining length scale of, combined reduced 4D 13C exchange and 1H spin diffusion experiment for, Tracht et al., 140, 460

Dynamic nuclear polarization

¹H, at 1.4 T, water doped with triarylmethyl-based radical, Wind and Ardenkjær-Larsen, 141, 347

high-field, with multiple-frequency resonance structure, Weis et al., 140,

low-field pulsed, Alecci and Lurie, 138, 313

in pulsed ENDOR experiments, Kouskov et al., 137, 25

Dynamic processes

water molecules in tendon, ¹H and ²H homonuclear and heteronuclear MQF NMR, Eliav and Navon, 137, 295

Dynamics

and origin of residual NMR linewidth of peptide bound to resin under MAS, Elbayed et al., 136, 127

parameters, estimation from NMR relaxation data using Lipari-Szabo model-free approach and Bayesian statistical methods, Andrec, Montelione, and Levy, 139, 408

Ε

Earth's magnetic field

self-diffusion imaging by spin echo, Mohorič et al., 136, 22

Echo planar imaging

NMR microscopy using, resolution, Peters and Bowtell, 137, 196 porous media, with spatial resolution below 100 µm, Manz, Chow, and Gladden, 136, 226

E.COSY

2D ω_1 -filtered, J-coupling crosstalk artifacts in, estimation with PFG- ω_1 filtered TOCSY, Xu, Zhang, and Evans, 138, 127

measurement of magnitude and sign of heteronuclear coupling constants in transition metal complexes, Otting, Soler, and Messerle, 137, 413; erratum, 139, 186

Edge enhancement

MRI, as diffusive discord of spin phase structure, Stepišnik et al., 137, 154

¹³C CPMAS, methylene-only subspectra using double-quantum filtering sequence, Rossi, Subramanian, and Harbison, 141, 159

chemical exchange-relaved NOEs in NMR experiments for observation of protein-water interactions, Melacini, Kaptein, and Boelens, 136, 214 computer-assisted assignment of 13C or 15N edited 3D-NOESY-HSQC

spectra using back-calculated and experimental spectra, Görler et al., **137.** 39

MUSIC in triple-resonance experiments: amino acid type-selective ¹H–¹⁵N correlations, Schubert et al., 141, 34

¹⁵N-edited 3D ROESY and NOESY HMQC and HSQC, signal enhancement using 45° water flipback for, Gruschus and Ferretti, 140, 451

Elastomers

crosslinked, redisual dipolar couplings in, 1H NMR imaging, Schneider, Demco, and Blümich, 140, 432

Electrically detected magnetic resonance (EDMR)

signal intensity, at resonant frequencies from 300 to 900 MHz in constant microwave field, Sato et al., 139, 422

Electric current

induced magnetic resonance phase imaging, Bodurka et al., 137, 265 Electric field

transversely oriented, tunable reentrant resonator with, for in vivo EPR spectroscopy, Chzhan et al., 137, 373

Electromagnetic detection

and micromechanical detection, simultaneous, in EPR, Alzetta et al., 141,

Electron nuclear double resonance spectroscopy (see ENDOR; Pulsed ENDOR)

Electron spin echo

absolute signal and noise intensities, Rinard et al., 140, 69

decay, of X-irradiated ammonium tartrate, Brustolon, Zoleo, and Lund, 137,

Electron spin echo envelope modulation (see ESEEM)

Electron spin echo spectrometer

using far infrared lasers as excitation sources, principles and performance, Moll et al., 137, 46

Electron spin lattice relaxation rates

for $S = \frac{1}{2}$ molecular species in glassy matrices or magnetically dilute solids, temperatures 10-300 K, Zhou et al., 139, 165

Electron spin quantum number

 $S = \frac{5}{2}$, low-symmetry complexes, paramagnetic proton nuclear spin relaxation theory of, Strandberg and Westlund, 137, 333

Electron spin transition

solution applicable to ensemble of isolated electrons, Boyd, 139, 109

Electrophoretic NMR capillary array, of proteins in biological buffer solutions, He et al., 141, 355

high-field, with multiple-frequency resonance structure, Weis et al., 140,

293

non-Kramers, S=2 ferrous ion of [Fe(II)EDTA]²⁻, Song *et al.*, **141**, 291 pulsed ENDOR experiments, dynamic nuclear polarization in, Kouskov *et al.*, **137**, 25

Enzyme-substrate interactions

paramagnetic effects on nuclear relaxation in enzyme-bound Co(II)-adenine nucleotide complexes, role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

EPI

NMR microscopy using, resolution, Peters and Bowtell, **137**, 196 signal intensities in FLASH-EPI-Hybrid sequences, Hillenbrand *et al.*, **139**, 74

EPR

absolute EPR spin-echo and noise intensities, Rinard *et al.*, **140**, 69 electrically detected MR signal intensities at resonant frequencies from 300 to 900 MHz in constant microwave field, Sato *et al.*, **139**, 422

electron spin transition solution applicable to ensemble of isolated electrons, Boyd. **139**, 109

high-frequency, 139.5-GHz, nitroxide side-chain dynamics in helix-forming peptide revealed by, Bennati et al., 139, 281

in vivo, tunable reentrant resonator with transverse orientation of electric field for, Chzhan et al., 137, 373

polycrystalline spectrum, evaluation of spin-Hamilltonian parameters and linewidth from, Misra, **140**, 179

powder spectra, modeling using numerical diagonalization of spin Hamiltonian, Morin and Bonnin, **136**, 176

signal-to-noise, frequency dependence, Rinard et al., 140, 218

simultaneous observation by micromechanical and electromagnetic methods, Alzetta et al., 141, 148

spectra, angular variation: simulation of polycrystalline EPR spectrum, Misra, 137, 83

transient MR without RF field pulses: fast field switching, Sloop, Lin, and Ackerman, 139, 60

EPR dosimeter

spin concentration: electron spin echo study of X-irradiated ammonium tartrate, Brustolon, Zoleo, and Lund, 137, 389

EPR probe

Q-band, for quantitative studies of even-electron metalloproteins, Petasis and Hendrich, 136, 200

EPR spin labels

in liquids, linewidth analysis

experimental, Robinson, Mailer, and Reese, 138, 210

theory and data analysis, Robinson, Mailer, and Reese, 138, 199

nitroxide, helix-forming peptide labeled with, nitroxide side-chain dynamics by high-frequency EPR, Bennati *et al.*, **139**, 281

Equilibrium density matrix,

significance of higher-order terms: multiple spin echoes, multiple quantum coherence, and dipolar field: Minot, Callaghan, and Kaplan, **140**, 200

Erythrocyte membranes

unsealed and cytoskeleton-depleted, competition between Na⁺ and Li⁺:
²³Na MQF and ⁷Li relaxation study, Srinivasan *et al.*, **140**, 206

Erythrocyte suspensions

assignment of coherence features in NMR *q*-space plots to particular diffusion modes in, Torres *et al.*, **138**, 135

ESEEM

absolute-value spectra, dead time-dependent line distortions in, Van Doorslaer, Sierra, and Schweiger, 136, 152

 14 N (I = 1), general analysis, Lee, Doan, and Hoffman, **140**, 91

non-Kramers, S = 2 ferrous ion of [Fe(II)EDTA]²⁻, Song *et al.*, **141**, 291 pure absorption ESEEM spectra using filter-diagonalization method for harmonic inversion, Jeschke, Mandelshtam, and Shaka, **137**, 221

ESR (see EPR)

Evolution strategy

optimization, for adiabatic pulses in MRI, Lunati et al., 138, 48

Exchange NMR

combined reduced 4D ¹³C exchange and ¹H spin diffusion experiment for determining length scale of dynamic heterogeneities, Tracht *et al.*, **140**, 460

1D solid-state MAS, superslow backbone protein dynamics study, Krushelnitsky et al., 138, 244

Exchange sample-turning NMR

²H 1D, application of narrowband excitation of ²H powder pattern, Reichert *et al.*, **139**, 308

Excitation bandwidth

calculations of multipulse sequence in NQR of spins $\frac{3}{2}$, Odin, 141, 239 Excitation sculpting

and PFGSE, band-selective HSQC and HMBC experiments using, Gaillet *et al.*, **139**, 454

quantitative measurement of long-range nuclear Overhauser enhancements, Harris et al., **140**, 504

with single axis gradients, unwanted signal leakage in, Jerschow, 137, 206 exercise

effect on creatine resonances in ¹H MR spectra of human skeletal muscle, Kreis *et al.*, **137**, 350

Exponential time-cubed echo delays

conditions for, Pfitsch, McDowell, and Conradi, 139, 364

External unit

low-frequency ¹H NMR, for analysis of large foodstuff samples, Capozzi *et al.*, **138**, 277

Extrapolation

transforming NMR data despite missing points, Kuethe et al., 139, 18

F

 ^{19}F

-13C distances, in p-trifluoromethylphenyl[1,2-13C₂]acetate, REDOR-determined, Schaefer, 137, 272

5-fluorouracil catabolism in liver: spectral decomposition using bilinear Bayesian approach, Ochs *et al.*, **137**, 161

and ¹H, cross-polarization dynamics between, analysis based on spin thermodynamics theory, Ando, Harris, and Reinsberg, **141**, 91

homonuclear dipolar couplings, structural parameters by multipulse solidstate NMR on static and oriented systems, Grage and Ulrich, **138**, 98 solid-state NMR magic-angle-turning experiments with multiple-pulse homonuclear decoupling, Hughes, Brouwer, and Harris, **138**, 256

sulfur hexafluoride, gas MRI: single-point ramped imaging with T_1 enhancement (SPRITE), Prado *et al.*, **137**, 324

two-dimensional NMR of oxyfluorides, high-order spin diffusion mechanisms in, Du, Levitt, and Grey, **140**, 242

Far infrared lasers

electron spin echo spectrometer using, principles and performance, Moll et al., 137, 46

Fast-DENSE

high-resolution strain analysis of human heart, Aletras, Balaban, and Wen, $\mathbf{140.}\ 41$

Fast imaging

brain metabolites, using double echo-filter metabolite imaging technique, Chen and Hu, **140**, 363

simple reliable solutions for spiral MRI gradient design, Salustri, Yang, and Glover, **140**, 347

Fast spin-echo imaging

effects of J coupling, density matrix simulations, Stables *et al.*, **140**, 305 Fat suppression

J coupling-induced, in DIET imaging, Stables et al., 136, 143

Feedback control

optimization of offset frequency in SORC sequence, Blauch, Schiano, and Ginsberg, 139, 139

optimization of pulse width in SORC sequence, Schiano et al., 140, 84

[Fe(II)EDTA]2-

S = 2, non-Kramers ENDOR and ESEEM, Song et al., 141, 291

Ferrocytochrome

protein hydration study using slaved pulses, Bornet, Guerlesquin, and Piotto, 138. 107

Ferroelectric

RbH₂PO₄, ⁸⁷Rb spin diffusion studied by 2D exchange NMR, Cereghetti and Kind. **138**, 12

Feruloylarabinoxylane

band-selective HSQC and HMBC experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

Filling factor

birdcage coils, Doty et al., 138, 144

Films

planar, profiling, high-gradient permanent magnet for, Glover et al., 139, 90 Filter-diagonalization method

for harmonic inversion, pure absorption ESEEM spectra using, Jeschke, Mandelshtam, and Shaka, 137, 221

Filtering

double-quantum filtering sequence, methylene-only subspectra in ¹³C CP MAS using, Rossi, Subramanian, and Harbison, **141**, 159

low-pass, elimination of artifacts introduced by zero-order phase correction in ¹H NMR, Wild, **137**, 430

X/¹H, suppression of ABX strong coupling signals in heteronuclear scalar and dipolar correlation spectra, Kövér and Batta, **138**, 89

Filters

spin-state-selective, double-/zero-quantum 2D NMR spectra simplified by, in measurement of homonuclear ²*J*-couplings, Permi *et al.*, **139**, 273

Finite impulse response filter

for solvent suppression, for accurate quantification of ¹H spectra, Sundin *et al.*, **139**, 189

First directional derivative

comparison of measurement schemes for cross-relaxation rate constant between two spins, Boulat, 139, 354

Fitting

EPR powder spectra, using numerical diagonalization of spin Hamiltonian, Morin and Bonnin, 136, 176

FK506 binding protein

complexed to FK506, H^N-H^α residual dipolar couplings in, measurement, Cai et al., 139, 451

FLASH

functional MR imaging of human brain using, effects of imaging parameters, Preibisch and Haase, 140, 162

FLASH-EPI-Hybrid sequences

signal intensities in, Hillenbrand et al., 139, 74

FLASH imaging

fast NMR flow measurements in plants using, Rokitta, Zimmermann, and Haase, 137, 29

Flow

fast NMR measurements in plants using FLASH imaging, Rokitta, Zimmermann, and Haase, 137, 29

Flow EPR

rapid scan, dielectric resonator-based, Sienkiewicz et al., 136, 137

Flow relaxivity

elucidation using flow relaxography, Lee et al., 136, 102

Flow relaxography

elucidation of flow relaxivity using, Lee et al., 136, 102

Fluid transport

time correlations in, obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

Fluoropolymer

analysis of cross-polarization dynamics between ¹⁹F and ¹H based on spin thermodynamics theory, Ando, Harris, and Reinsberg, **141**, 91

5-Fluorouracil

catabolism in human liver, ¹⁹F nonlocalized study: spectral decomposition using bilinear Bayesian approach, Ochs *et al.*, **137**, 161

fMRI (see Magnetic resonance imaging, fMRI)

Foodstuffs

large samples, low-frequency ¹H NMR external unit for analysis of, Capozzi et al., **138**, 277

Four-dimensional NMR

combined reduced 4D ¹³C exchange and ¹H spin diffusion experiment for determining length scale of dynamic heterogeneities, Tracht *et al.*, **140**, 460

high-resolution HMQC-NOESY-HSQC spectroscopy, Morshauser and Zuiderweg, **139**, 232

Frequency dependence

EPR signal-to-noise, Rinard et al., 140, 218

Frequency domain

reference deconvolution in, Goez and Heun, 136, 69

Frequency-modulated pulse

composite pulsed field gradients with refocused chemical shifts and short recovery time, Hu and Shaka, 136, 54

Frictional heating

temperature calibration under ultrafast MAS conditions, Langer *et al.*, **138**, 182

Full relaxation matrix approach

computer-assisted assignment of ¹³C or ¹⁵N edited 3D-NOESY–HSQC spectra using back-calculated and experimental spectra, Görler *et al.*, **137**, 39

G

GAMMA

spectral simulations incorporating gradient coherence selection, Young et al., 140, 146

Gas flow imaging

MRI, using circulating laser-polarized ¹²⁹Xe, Brunner et al., 138, 155

Gas imaging

single-point ramped imaging with T_1 enhancement (SPRITE) MRI, Prado et al., 137, 324

Gelatin gels

state of water in, NMR relaxation study, Vackier, Hills, and Rutledge, 138, 36

Glass

chemical bonding of lead in, analysis with isotropic vs anisotropic correlation: PASS shifted echo, Fayon *et al.*, **137**, 116

magnesium aluminoborate, $^{11}B\{^{27}Al\}$ high-resolution heteronuclear correlation spectrum, Chan, 140, 487

Glassy matrices

 $S=\frac{1}{2}$ molecular species in, electron spin lattice relaxation rates at temperatures 10–300 K, Zhou *et al.*, **139**, 165

Glassy solution

chromium(V) and vanadyl complexes in, spin-echo dephasing for, solvent and temperature dependence, Eaton and Eaton, 136, 63

Glucose

aqueous solution, high-resolution NMR, suppression of radiation damping, Barjat, Mattiello, and Freeman, 136, 114

Glutamate

cerebral concentrations, *in vivo* quantitation using natural abundance ¹³C MRS at 1.5 T, Blüml, **136**, 219

Glutamine

cerebral concentrations, *in vivo* quantitation using natural abundance ¹³C MRS at 1.5 T, Blüml, **136**, 219

Glycin

alpha protons, selective correlation of amide groups in proteins to, by multiple-quantum spectroscopy, Bazzo, Cicero, and Barbato, 136, 15

Glycoconjugates

band-selective HSQC and HMBC experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

g-matrix

based on configuration interaction and Stone's perturbation theory, Li et al., 138, 74

Gradient BIRD_R

for selection of uncoupled magnetization, Heikkinen and Kilpeläinen, 137, 93

Gradient coherence selection

spectral simulations incorporating, Young et al., 140, 146

transverse relaxation-optimized gradient-enhanced triple-resonance NMR spectroscopy, Loria, Rance, and Palmer, 141, 180

Gradient coil:

magic angle, target field design for, Barbara and Bronnimann, **140**, 285 real, reconstructing powder NQR images with, Swaminathan and Suits, **138**, 123

Gradient coil set

biplanar, fast optimization, Tomasi et al., 140, 325

Gradient echo slice excitation profile imaging (GESEPI)

microimaging at 14 T using, for removal of magnetic susceptibility artifacts in T**-weighted image contrast, Yang et al., 141, 1

Gradients (see also Pulsed-field gradients)

local magnetic susceptibility-induced, effects on water diffusion measurements in brain *in vivo*, Clark, Barker, and Tofts, **141**, 52

magnetic field, in solid-state MAS NMR, Maas et al., 141, 29

orthogonal high-strength, permanent magnet with, for profiling of planar films and coatings, Glover et al., 139, 90

spiral MRI, design, simple reliable solutions for, Salustri, Yang, and Glover, **140**, 347

temperature, and convection, measurement in liquid samples, Loening and Keeler, 139, 334

Gradient set

high-strength openable, for orthopedic MRI, Crozier et al., 139, 81 Gradient spin echo

of restricted diffusion: MRI edge enhancement as diffusive discord of spin phase structure, Stepišnik et al., 137, 154

Gradient waveforms

generalized, spin echo analysis of restricted diffusion in porous media under, Codd and Callaghan, **137**, 358

Guanidine groups

arginine side chains, correlation to delta protons by multiple quantum spectroscopy, Bazzo, Cicero, and Barbato, 136, 15

g values

halomolybdenyl, -vanadyl, and -chromyl complexes, Li et al., 138, 80

Н

²H

glycerol-d8 in DMSO-d6, relaxation effects in system of spin- $\frac{1}{2}$ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali. 136, 27

²H, ¹³C, ¹⁵N-labeled proteins, observation of through-hydrogen-bond ^{2h}J_{HC}, Cordier et al., **140**, 510

MAS NMR spectra, separation by 2D spectroscopy, Kristensen et al., 139, 314

powder pattern, narrowband excitation and application to ²H 1D exchange sample-turning NMR, Reichert *et al.*, **139**, 308

(HACACO)NH

2D J^{CH} -modulated pulse scheme for quantitative measurement of $^{13}\text{C}^{\alpha-1}\text{H}^{\alpha}$ couplings in ^{15}N , ^{13}C -labeled proteins, Hitchens, McCallum, and Rule, 140, 281

Halochromyl complexes

g values, Li et al., 138, 80

Halomolybdenyl complexes

g values, Li et al., 138, 80

Halovanadyl complexes

g values, Li et al., 138, 80

Harmonic inversion

by filter-diagonalization method, pure absorption ESEEM spectra using, Jeschke, Mandelshtam, and Shaka, 137, 221

Hartmann-Hahn match conditions

for CP/MAS between two half-integer quadrupolar nuclei, examples, East-man, 139, 98

Hartmann-Hahn transfer

single-shot experiments for acquisition of coherence-transfer functions in real time, Luy and Glaser, 138, 187

HBHA(CBCACO)NH

multi-quantum version with enhanced sensitivity for partially deuterated samples, Gschwind, Kessler, and Gemmecker, 137, 285

HCCCH experiment

for through-bond correlation of thymine resonances in ¹³C-labeled DNA oligonucleotides, Sklenář, Masse, and Feigon, **137**, 345

HCCH

three-dimensional TROSY-type NMR correlation of aromatic ¹H-¹³C groups in proteins, optimization, Meissner and Sørensen, **139**, 447

³H

hyperpolarized, MRI, quantification of regional intrapulmonary oxygen partial pressure evolution during apnea, Deninger *et al.*, **141**, 207

laser-polarized

single-shot diffusion measurement in, Peled *et al.*, **140**, 320 system for low-field imaging, Wong *et al.*, **141**, 217

Head

immobilization: integrated system with high-performance RF coil for fMRI of visual paradigms at 1.5 T (human), Thulborn and Shen, 139, 26

 $^{31} P$ CSI study: spectral decomposition using bilinear Bayesian approach (human), Ochs *et al.*, 137, 161

Heart

functional MRI, displacement encoding with stimulated echoes (beagle, human): DENSE, Aletras *et al.*, **137**, 247

high-resolution strain analysis with fast-DENSE (human), Aletras, Balaban, and Wen, 140, 41

НЕНАНА

single-shot experiments for acquisition of coherence-transfer functions in real time, Luy and Glaser, ${\bf 138}$, ${\bf 187}$

3Helium

thermally polarized gas, NMR imaging, Kober *et al.*, **138**, 308

Q-band EPR probe for quantitative studies of, Petasis and Hendrich, 136, 200

Heteronuclear chemical-shift correlation

band-selective HSQC and HMBC experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

Heteronuclear correlation

experimental aspects of multidimensional solid-state NMR correlation spectroscopy, Ramamoorthy, Wu, and Opella, **140**, 131

H5 and exchangeable pyrimidine base hydrogens in ¹³C, ¹⁵N-labeled RNA, triple-resonance experiments for, Wöhnert *et al.*, **139**, 430

high-resolution, between quadrupolar nuclei, Chan, **140**, 487 multiple-quantum (*see* HMQC)

scalar and dipolar, suppression of ABX strong coupling signals in, Kövér and Batta, 138, 89

and sensitivity improvement of TROSY, Rance, Loria, and Palmer, **136**, 92 single-quantum (*see* HSQC)

solid-state wideline, isotropic mixing, sign discrimination, and sensitivity in, Oliver and Titman, **140**, 235 Heteronuclear decoupling

and anomalous rotational resonance spectra in MAS NMR, Helmle et al., **140,** 379

Heteronuclear relaxation

bias estimation: method for determining B_1 field inhomogeneity, Guenneugues, Berthault, and Desvaux, 136, 118

Heteronuclear triple-quantum-filtered NMR

dipolar interactions and dynamic processes of water in tendon, Eliav and Navon, 137, 295

Higher-order gradients

beyond k-space: SLOOP^N, Pohmann, Rommel, and von Kienlin, 141, 197 Higher-order terms

in equilibrium density matrix, significance: multiple spin echoes, multiple quantum coherence, and dipolar field: Minot, Callaghan, and Kaplan,

High fields

simultaneous micromechanical and electromagnetic detection in EPR, Alzetta et al., 141, 148

High-frequency EPR

139.5-GHz, nitroxide side-chain dynamics in helix-forming peptide revealed by, Bennati et al., 139, 281

High-resolution magnetic relaxation dispersion

solute spin probes, using dual-magnet system, Wagner et al., 140, 172 High-resolution NMR

signal selection by pulsed-field gradients

design of gradient pulse sequences, Thomas et al., 137, 10 geometrical analysis, Mitschang, 137, 1

spectrometer: mapping B_1 field distribution with nonideal gradients, Jerschow and Bodenhausen, 137, 108

suppression of radiation damping, Barjat, Mattiello, and Freeman, 136, 114 with z-axis pulsed-field gradients, simulations, Meresi et al., 137, 186 High-salt solutions

biological buffer solutions, capillary array electrophoretic NMR of proteins in, He et al., 141, 355

Histidine-containing phosphocarrier protein

computer-assisted assignment of 13C or 15N edited 3D-NOESY-HSQC spectra using back-calculated and experimental spectra, Görler et al., **137,** 39

HIV protease

perdeuterated. ¹H-¹⁵N correlated ¹H CPMG experiments, transverse ¹H cross relaxation in, Ishima, Louis, and Torchia, 137, 289

band-selective experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

HMOC

constant-time, determination of ${}^{3}J(H3'_{i}, P_{i+1})$ and ${}^{3}J(H5'_{i}/5''_{i}, P_{i})$ coupling constants in 13C-labeled nucleic acids, Hu et al., 139, 181

detection of intermolecular chemical exchange through decorrelation of two-spin order, Skrynnikov and Ernst, 137, 276

dipolar

¹H-¹³C multiple-quantum, with recoupled polarization transfer, in solids under ultra-fast MAS, Saalwächter, Graf, and Spiess, 140, 471

heteronuclear DQ MAS NMR, Saalwächter et al., 139, 287

with ISIS localization, in vivo detection of 15N-coupled protons in rat brain, Kanamori and Ross, 139, 240

pure-phase homonuclear J-modulated, with tilted cross-peak patterns, for accurate determination of homonuclear coupling constants, Koźmiński, **141,** 185

sensitivity-enhanced sim-CT HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH triple-resonance experiments, Swapna and Montelione,

3D ¹⁵N-edited ROESY and NOESY experiments, signal enhancement using 45° water flipback, Gruschus and Ferretti, 140, 451

2D {31P} spin-echo-difference constant-time [13C, 1H] HMQC experiment for simultaneous determination of ${}^3J_{\text{H3'P}}$ and ${}^3J_{\text{C4'P}}$ in ${}^{13}\text{C-labeled}$ nucleic acids and protein complexes, Szyperski et al., 140, 491

HMQC-NOESY-HSQC

high-resolution 4D experiment, Morshauser and Zuiderweg, 139, 232 $HN(\alpha/\beta\text{-COCA-}J)$

measurement of ¹J_{C'Cα} couplings from 2D [¹⁵N, ¹H] correlation spectrum, Permi et al., 141, 44

Homonuclear decoupling

sequence: off-resonance dynamics and coherent averaging theory, Cho, 141, 164

Homonuclear experiments

quantitative fully J-decoupled homonuclear NMR spectra: obtaining pure absorption 2D J-spectra, Mutzenhardt, Guenneau, and Canet, 141, 312 Homonuclear triple-quantum-filtered NMR

dipolar interactions and dynamic processes of water in tendon, Eliav and Navon, 137, 295

Homotopy matrix diagonalization

in simulation of polycrystalline EPR spectrum, Misra, 137, 83 **HSOC**

band-selective experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

J-multiplied: method for measurement of ³J (H_NH_α) couplings in ¹⁵Nlabeled proteins, Heikkinen et al., 137, 243

and J spectroscopy, in separate quantification of double and singly ¹³Clabeled metabolites, Davison, Jones, and Dixon, 137, 448

MUSIC in triple-resonance experiments: amino acid type-selective ¹H⁻¹⁵N correlations, Schubert et al., 141, 34

sensitivity-enhanced, artifacts in, Turner, Connolly, and Stern, 137, 281 spin-state-selective TPPI: suppression of heteronuclear coupling constants in multidimensional NMR, Schulte-Herbrüggen et al., 139, 443

3D 15N-edited ROESY and NOESY experiments, signal enhancement using 45° water flipback, Gruschus and Ferretti, 140, 451

HSOC-TOCSY

simplified multiplet pattern, for determination of long-range heteronuclear coupling constants, Koźmiński, 137, 408

Hybrid imaging

signal intensities: FLASH-EPI-Hybrid sequences, Hillenbrand et al., 139, 74 Hybrid numerical method

asymmetric MRI magnet design using, Zhao, Crozier, and Doddrell, 141,

Hydration

NMR experiments for observation of protein-water interactions, editing of chemical exchange-relayed NOEs in, Melacini, Kaptein, and Boelens,

Hydroxyaluminum diacetate

¹³C-²⁷Al dipolar interactions in, ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of, van Wüllen and Kalwei, 139, 250

Hypercomplex spectroscopy

separation of ²H MAS NMR spectra by 2D spectroscopy, Kristensen et al., **139.** 314

Hyperpolarized ³He

MRI, quantification of regional intrapulmonary oxygen partial pressure evolution during apnea, Deninger et al., 141, 207

Hyperpolarized ¹²⁹Xe

MRI, implications of role of oxygenation in T_1 of 129 Xe in blood, Albert etal., 140, 264

single-shot diffusion measurement in, Peled et al., 140, 320

Image artifacts

magnetic susceptibility artifacts in T_2^* -weighted image contrast, microimaging at 14 T using GESEPI for removal of, Yang et al., 141, 1

ı

Image reconstruction

powder NQR images, with real gradient coils, Swaminathan and Suits, 138, 123

Image-selected in vivo spectroscopy (ISIS)

with HMQC, in *in vivo* detection of ¹⁵N-coupled protons in rat brain, Kanamori and Ross, **139**, 240

Imaging

DIET, J coupling-induced fat suppression in, Stables et al., 136, 143

¹H NMR, of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, 140, 432

parameters, effects on functional MR imaging of human brain using FLASH, Preibisch and Haase, **140**, 162

powder NQR, image reconstruction with real gradient coils, Swaminathan and Suits, 138, 123

RF time-domain EPR, high-speed data acquisition system and receiver configurations for, Subramanian et al., 137, 379

selective, of biofilms in porous media, by NMR relaxation, Hoskins *et al.*, **139.** 67

self-diffusion, by spin echo in Earth's magnetic field, Mohorič *et al.*, **136**, 22 spin-echo and fast spin-echo, effects of *J* coupling in, density matrix simulations, Stables *et al.*, **140**, 305

Immobilization

head, integrated system with high-performance RF coil for fMRI of visual paradigms at 1.5 T, Thulborn and Shen, 139, 26

IMPEACH-MBC

improved performance accordion heteronuclear multiple-bond correlation spectroscopy, Hadden, Martin, and Krishnamurthy, **140**, 274

NADEOUATE

solid-state dipolar spectra, with large double-quantum spectral width, Hong, 136, 86

INADEQUATE-CR

experiments in solid state, Verel, van Beek, and Meier, 140, 300

Indirect ¹³C imaging

mixing sequences for selective heteronuclear *J* cross polarization for: PRAWN, Chandrakumar and Kimmich, **137**, 100

INDO-CI-Stone model

g values of halomolybdenyl, -vanadyl, and -chromyl complexes, Li et al., 138, 80

INEPT

phase-sensitive 2D, accurate measurements of multiple-bond ¹³C-¹H coupling constants from, Ding, **140**, 495

Inhomogeneity effects

birdcage coils, Doty et al., 138, 144

Injection of magnetization

selective, by slow chemical exchange in NMR, Boulat, Epstein, and Rance, 138, 268

Instrumentation

transient MR without RF field pulses: fast field switching, Sloop, Lin, and Ackerman, 139, 60

Interaction representation formalism

calculations of multipulse sequence in NQR of spins $\frac{3}{2}$, Odin, 141, 239 Interactions

anisotropic spin, order matrix analysis of residual dipolar couplings using singular value decomposition, Losonczi *et al.*, **138**, 334

one-spin and two-spin, efficient refocusing for NMR quantum computation, Jones and Knill, **141**, 322

Interaction tensors

determined from rotational resonance MAS NMR lineshapes of four-¹³C-spin system, magnitudes and orientations of, Dusold, Maisel, and Sebald, **141**, 78

Inter-ligand Overhauser effect

theoretical analysis: mapping structural relationships of macromolecular ligands, London, **141**, 301

Intermolecular chemical exchange

detection through decorrelation of two-spin order, Skrynnikov and Ernst, 137, 276

Internal dynamics

ranalexin in water and TFE: quantitative measurement of longitudinal and transverse cross-relaxation rates, Malliavin et al., 140, 189

Internal gradients

diffusion measurements in presence of, PFGSE method, Sørland, Aksnes, and Gjerdåker, 137, 397

Inversion

NMR log data sets with different measurement errors, Dunn and LaTorraca, 140, 153

Ischemia

focal cerebral, murine models, application of high-resolution MR angiography of mouse brain, Beckmann, Stirnimann, and Bochelen, **140**, 442 ISIS (*see* Image-selected *in vivo* spectroscopy)

Isotope effects

on ¹⁷O, ¹H coupling constant and ¹⁷O–{¹H} NOE in water, Sergeyev, Sergeyeva, and Raynes, **137**, 311

Isotope filters

gradient $BIRD_{\mbox{\tiny R}}$ method for selection of uncoupled magnetization, Heikkinen and Kilpeläinen, ${\bf 137},\,93$

Isotropic/anisotropic shift correlation

in analysis of chemical bonding of lead in glasses: PASS shifted echo, Fayon et al., 137, 116

Isotropic mixing

analytical polarization transfer functions for four coupled spins $\frac{1}{2}$, Luy, Schedletzky, and Glaser, 138, 19

general AMX spin system under, analytical coherence-transfer functions for, Schedletzky and Glaser, **123A**, 174; *erratum*, **136**, 134

and sign discrimination and sensitivity, in solid-state wideline heteronuclear correlation experiments, Oliver and Titman, 140, 235

Isotropic weighting

optimized pulse sequence for diffusion-weighted imaging, Cercignani and Horsfield, ${\bf 140,}~58$

J

I^{CH}

 J^{CH} -modulated 2D (HACACO)NH pulse scheme for quantitative measurement of $^{13}\text{C}^{\alpha}$ - $^{1}\text{H}^{\alpha}$ couplings in ^{15}N , ^{13}C -labeled proteins, Hitchens, McCallum, and Rule, **140**, 281

J-coupling

crosstalk artifacts in 2D ω_1 -filtered E.COSY spectra, estimation with PFG- ω_1 -filtered TOCSY, Xu, Zhang, and Evans, 138, 127

effects in spin-echo and fast spin-echo imaging, density matrix simulations, Stables *et al.*, **140**, 305

efficient refocusing of one-spin and two-spin interactions for NMR quantum computation, Jones and Knill, 141, 322

homonuclear ²*J*-coupling, measurement from spin-state selective double-/ zero-quantum 2D NMR spectra, Permi *et al.*, **139**, 273

induced fat suppression in DIET imaging, Stables et al., 136, 143

 $^{1}J_{C'C\alpha}$ couplings, measurement from 2D [15 N, 1 H] correlation spectrum, HN(α/β -COCA-J) experiment for, Permi *et al.*, **141**, 44

³J_{H3'P} and ³J_{C4'P} in ¹³C-labeled nucleic acids and protein complexes, 2D { ³¹P} spin-echo-difference constant-time [¹³C,

¹H] HMQC experiment for simultaneous determination, Szyperski *et al.*, **140**, 491

 $^1J_{\rm NC'}$ and $^2J_{\rm H^NC'}$ couplings, measurement from spin-state selective 2D correlation spectrum, Permi *et al.*, **140**, 32

¹⁷O, ¹H in water, isotope effects, Sergeyev, Sergeyeva, and Raynes, **137**, 311 through-hydrogen-bond ^{2h}J_{HC}, observation in perdeuterated protein, Cordier *et al.*, **140**, 510

J-coupling constants

between 13 C $^{\alpha}$ or 1 H $^{\alpha}$ and other protons in protein, 13 C natural abundance S 3 E and S 3 CT experiments for measurement of, Sørensen, Meissner, and Sørensen, 137, 237

determination by deconvolution of multiplets in NMR, Jeannerat and Bodenhausen, 141, 133

heteronuclear, in transition metal complexes, measurement of magnitude and sign of, Otting, Soler, and Messerle, **137**, 413; *erratum*, **139**, 186 homonuclear, determination, pure-phase homonuclear *J*-modulated HMQC

experiment with tilted cross-peak patterns for, Koźmiński, **141**, 185

 $^{3}J(H3'_{i}, P_{i+1})$ and $^{3}J(H5'_{i}/5''_{i}, P_{i})$, determination in ^{13}C -labeled nucleic acids using CT-HMQC, Hu *et al.*, **139**, 181

 ^{3}J (H_NH_{α}) couplings in 15 N-labeled proteins, *J*-multiplied HSQC method for measurement of, Heikkinen *et al.*, **137**, 243

long-range heteronuclear, simplified multiplet pattern HSQC-TOCSY for determination, Koźmiński, 137, 408

long-range heteronuclear and homonuclear, PFG-ω₁-filtered TOCSY experiments for, Xu. Zhang, and Evans, 138, 127

multiple-bond ¹³C-¹H, accurate measurements from phase-sensitive 2D INEPT spectra, Ding, **140**, 495

one-bond ¹⁵N-¹H, in protein backbone, pulse sequences for measurement, Lerche *et al.*, **140**, 259

J pulses

for multiplet-selective NMR, Bendall and Skinner, 141, 261

J-scaling

with active-coupling-pattern tilting: pure-phase homonuclear *J*-modulated HMQC experiment for determination of homonuclear coupling constants, Koźmiński, **141**, 185

J spectroscopy

HSQC-filtered, in separate quantification of doubly and singly ¹³C-labeled metabolites, Davison, Jones, and Dixon, **137**, 448

obtaining pure absorption 2D *J*-spectra, Mutzenhardt, Guenneau, and Canet, **141**, 312

Κ

Knee

RARE images using openable high-strength gradient set (human), Crozier et al., 139, 81

triple-quantum-filtered twisted projection sodium MRI in vivo (human), Borthakur et al., **141**, 286

k-space

beyond k-space: spectral localization using higher-order gradients, Pohmann, Rommel, and von Kienlin, 141, 197

L

 ^{139}La

NMR, application of multiple-rotor-cycle QPASS pulse sequences, Aurentz et al., 138, 320

Lactate

simultaneous lactate editing and observation of other metabolites using stimulated-echo-enhanced double-quantum filter, Lei and Peeling, **137**, 215

in skeletal muscle, anisotropic orientation observed by dipolar coupling in ¹H NMR spectroscopy, Asllani *et al.*, **139**, 213

Lanthanide

chelates, as bilayer alignment tools in NMR studies of membrane-associated peptides, Prosser *et al.*, **141**, 256

paramagnetic ions, ¹³C MAS using, probing membrane surfaces and location of membrane-embedded peptides with, Gröbner, Glaubitz, and Watts, **141**, 335

Laponite

and saponite, suspensions, ⁷Li double-quantum filtered NMR and multinuclear relaxation rates, Grandjean and Robert, **138**, 43

Laser polarization

gas flow MRI using circulating laser-polarized ¹²⁹Xe, Brunner *et al.*, **138**, 155

system for low-field imaging of laser-polarized noble gas, Wong et al., 141, 217

Lasers

far infrared, electron spin echo spectrometer using, principles and performance, Moll et al., 137, 46

LCModel

in vivo quantification of 18 metabolites in short-echo-time ¹H NMR spectra of rat brain, Pfeuffer et al., **141**, 104

Lead

in glasses, chemical bonding through isotropic vs anisotropic correlation: PASS shifted echo, Fayon *et al.*, **137**, 116

Lectin

barley, residual dipolar couplings, order matrix analysis using singular value decomposition, Losonczi *et al.*, **138**, 334

Length scale

dynamic heterogeneities, combined reduced 4D ¹³C exchange and ¹H spin diffusion experiment for determining, Tracht *et al.*, **140**, 460

Li

and Na⁺, competition for unsealed and cytoskeleton-depleted human RBC membrane: ²³Na MQF and ⁷Li relaxation study, Srinivasan *et al.*, **140**, 206

7Li

double-quantum filtered NMR and multinuclear relaxation rates of clay suspensions, Grandjean and Robert, 138, 43

high-resolution magnetic relaxation dispersion measurements using dualmagnet system, Wagner et al., 140, 172

LiAlO₂, Hartmann-Hahn match conditions for CP/MAS between two halfinteger quadrupolar nuclei, Eastman, 139, 98

NMR relaxation evidence for competition between Na⁺ and Li⁺ for unsealed and cytoskeleton-depleted RBC membrane, Srinivasan *et al.*, **140**, 206

LiAlO₂

⁷Li and ²⁷Al, Hartmann–Hahn match conditions for CP/MAS between two half-integer quadrupolar nuclei, Eastman, **139**, 98

Lie algebra

and coherence transfer, in separation of ²H MAS NMR spectra by 2D spectroscopy, Kristensen *et al.*, **139**, 314

Ligands

macromolecular, mapping structural relationships: theoretical analysis of inter-ligand Overhauser effect, London, 141, 301

Limiter

microwave, cryogenically coolable, Rinard, Quine, and Eaton, 136, 207 Line broadening

origin of residual NMR linewidth of peptide bound to resin under MAS, Elbayed et al., 136, 127

Line narrowing

 $I=\frac{1}{2}$ spins coupled to quadruolar nuclei in liquids: effects of weak decoupling fields, Bendel and Baram, **141**, 121

Line scan imaging

single-shot, using stimulated echoes, Finsterbusch and Frahm, 137, 144 Lineshape

calculations, on spreadsheet software, Mayer, 138, 1

carbon-13, in 13 CD₂ spin grouping, cross-related quadrupolar spin relaxation and, Werbelow *et al.*, **140**, 1

rotational resonance MAS NMR, of four-¹³C-spin system, magnitudes and orientations of interaction tensors determined from, Dusold, Maisel, and Sebald, **141**, 78

and slow site exchange processes in solution NMR, Schurr et al., 140, 404 static powder, simulation, Ponti, 138, 288

Linewidth

from polycrystalline EPR spectrum, evaluation, Misra, 140, 179

residual NMR, of peptide bound to resin under MAS, origin of, Elbayed *et al.*, **136**, 127

Linewidth analysis

spin labels in liquids

experimental, Robinson, Mailer, and Reese, 138, 210

theory and data analysis, Robinson, Mailer, and Reese, 138, 199

Lipari-Szabo formalism

and Bayesian statistical methods, estimation of dynamic parameters from NMR relaxation data using, Andrec, Montelione, and Levy, **139**, 408 Liquid crystals

¹³C NMR with proton homonuclear dipolar decoupling methods, Fung, Ermolaev, and Yu, 138, 28

Liquid

comparison of experimental CSA methods in, Batta, Kövér, and Kowalewski, 136, 37

measurement of convection and temperature profiles in, Loening and Keeler, 139, 334

NMR, experimental control of spin diffusion, comparison of methods, Boulat, 139, 354

quadrupolar nuclei in, line narrowing of $I = \frac{1}{2}$ spins coupled to, effects of weak decoupling fields, Bendel and Baram, 141, 121

spin labels in, linewidth analysis

experimental, Robinson, Mailer, and Reese, 138, 210

theory and data analysis, Robinson, Mailer, and Reese, 138, 199

Litz coils

error-tolerant RF coils for NMR/MRI, Doty, Entzminger, and Hauck, 140, 17

Liver

5-fluorouracil catabolism, ¹⁹F nonlocalized study: spectral decomposition using bilinear Bayesian approach, Ochs *et al.*, **137**, 161

Localized spectroscopy

beyond k-space: spectral localization using higher-order gradients, Pohmann, Rommel, and von Kienlin, 141, 197

stimulated anti-echo selection in, Zhu and Smith, 136, 1

Log data sets

NMR, with different measurement errors, inversion of, Dunn and LaTorraca, 140, 153

Logic gates

NMR quantum, construction and implementation for two-spin systems, Price et al., 140, 371

Longitudinal magnetization

dipolar-encoded, based filter for ¹H NMR imaging of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, **140**, 432

Long-range heteronuclear shift correlation

improved performance accordion heteronuclear multiple-bond correlation spectroscopy: IMPEACH-MBC, Hadden, Martin, and Krishnamurthy, **140**, 274

Low magnetic field

system for low-field imaging of laser-polarized noble gas, Wong $\it et al., 141, 217$

Low-pass filtering

elimination of artifacts introduced by zero-order phase correction in ¹H NMR, Wild, **137**, 430

Low-symmetry complexes

electron spin quantum number $S=\frac{5}{2}$, paramagnetic proton nuclear spin relaxation theory, Strandberg and Westlund, 137, 333

Lung imaging

laser-polarized noble gas, low magnetic field (rat), Wong *et al.*, **141**, 217 quantification of regional intrapulmonary oxygen partial pressure evolution during apnea by ³He MRI (human, pig), Deninger *et al.*, **141**, 207 thermally polarized ³He gas (rat), Kober *et al.*, **138**, 308

M

Macromolecular ligands

mapping structural relationships: theoretical analysis of inter-ligand Overhauser effect, London, **141**, 301

Macromolecules

isotopically labeled

excitation of selected proton signals in, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

identification of spin diffusion pathways in, Eykyn, Früh, and Bodenhausen, 138, 330

offset profiles of selective pulses in, Eykyn, Ghose, and Bodenhausen, 136, 211

resonances, suppression in short-echo-time ¹H NMR spectroscopy of human brain, application of multiple inversion recovery, Knight-Scott, **140**, 228

resonances with short T_1 , role in underlying baseline resonances in rat brain: quantification of metabolites in short-echo-time ¹H NMR spectra, Pfeuffer *et al.*, **141**, 104

TROSY, sensitivity improvement, Rance, Loria, and Palmer, 136, 92 Magic-angle gradient coils

target field design for, Barbara and Bronnimann, 140, 285

Magic-angle spinning

anomalous rotational resonance spectra in, Helmle et al., 140, 379

¹³C, using lanthanide ions, probing membrane surfaces and location of membrane-embedded peptides with, Gröbner, Glaubitz, and Watts, 141, 335

 $^{13}\text{C}{^-}^2\text{D}$ dipolar interactions during, comparison of REDOR and θ -REDOR for measuring, Gullion, **139**, 402

with composite RF pulses, Leppert, Heise, and Ramachandran, **139**, 382 CP-MAS (*see* Cross polarization–magic-angle spinning)

dual processing of 2D exchange data in, Tycko and Berger, **141**, 141 fast, spin counting with, Geen *et al.*, **138**, 167

¹⁹F 2D NMR of oxyfluorides, high-order spin diffusion mechanisms in, Du, Levitt, and Grey, **140**, 242
heteronuclear double-quantum MAS NMR spectroscopy in dipolar solids,

Saalwächter *et al.*, **139**, 287 high-resolution, origin of residual NMR linewidth of peptide bound to resin,

Elbayed *et al.*, **136**, 127

²H MAS NMR spectra, separation by 2D spectroscopy, Kristensen *et al.*, **139**, 314

magnetic field gradients in, Maas et al., 141, 29

multiple-quantum, high-resolution heteronuclear correlation between quadrupolar nuclei, Chan, **140**, 487

1D solid-state MAS exchange NMR spectroscopy, superslow backbone protein dynamics study, Krushelnitsky et al., 138, 244

3PbO-2P₂O₅ glass, in analysis of chemical bonding of lead via isotropic vs anisotropic correlation: PASS shifted echo, Fayon *et al.*, **137**, 116

rotational resonance MAS NMR lineshapes of four-¹³C-spin system, magnitudes and orientations of interaction tensors determined from, Dusold, Maisel, and Sebald, **141**, 78

slow, 2D exchange NMR spectra under, Ernst, Kentgens, and Meier, **138**, 66 spectra, calculation influenced by slow molecular tumbling, Mayer, **139**, 132 target field design for magic angle gradient coils, Barbara and Bronnimann, **140**, 285

ultrafast

recoupled polarization transfer heteronuclear ¹H–¹³C multiple-quantum correlation in solids in, Saalwächter, Graf, and Spiess, **140**, 471 temperature calibration in, Langer *et al.*, **138**, 182

Magic-angle turning

¹³C and ¹⁵N, with TPPM decoupling, resolution enhancement in, McGeorge, Alderman, and Grant, 137, 138

¹⁹F solid-state NMR experiments with multiple-pulse homonuclear decoupling, Hughes, Brouwer, and Harris, 138, 256

Magic echo imaging

solid-state NMR imaging without rapidly switchable field gradient, Matsui et al., 138, 220

Magnesium aluminoborate glass

¹¹B{²⁷Al} high-resolution heteronuclear correlation spectrum, Chan, 140, 487

Magnet

high-gradient permanent, for profiling of planar films and coatings, Glover et al., 139, 90

MRI, asymmetric design using hybrid numerical method, Zhao, Crozier, and Doddrell, **141**, 340

Magnetic field

induced, in trabecular bone, evaluation of surface charge method for computing, Hwang and Wehrli, 139, 35

Magnetic field gradients

in solid-state MAS NMR, Maas et al., 141, 29

Magnetic relaxation dispersion

high-resolution, measurements of solute spin probes, using dual-magnet system, Wagner et al., **140**, 172

Magnetic resonance angiography

high-resolution, of mouse brain, application to focal cerebral ischemia models, Beckmann, Stirnimann, and Bochelen, **140**, 442

Magnetic resonance imaging

adiabatic pulses in, evolution strategy optimization for, Lunati *et al.*, **138**, 48 asymmetric magnet design using hybrid numerical method, Zhao, Crozier, and Doddrell, **141**, 340

current density imaging of chemical processes and reactions, Beravs, Demšar, and Demsar, 137, 253

current-induced MR phase imaging, Bodurka et al., 137, 265

diffusion tensor

comparison of acquisition schemes for, Papadakis *et al.*, **137**, 67 comparison of scalar measures used in, Bahn, **139**, 1

invariant and orthonormal scalar measures derived from, Bahn, **141**, 68 edge enhancement, as diffusive discord of spin phase structure, Stepišnik *et al.*, **137**, 154

effects of local magnetic susceptibility-induced gradients on water diffusion measurements in brain *in vivo*, Clark, Barker, and Tofts, **141**, 52

error-tolerant RF Litz coils for, Doty, Entzminger, and Hauck, **140**, 17 fast-DENSE high-resolution strain analysis of human heart, Aletras, Balaban, and Wen, **140**, 41

fMRI

brain, using FLASH, effects of imaging parameters (human), Preibisch and Haase, 140, 162

cardiac, displacement encoding with stimulated echoes in: DENSE, Aletras et al., 137, 247

with hyperpolarized ³He, quantification of regional intrapulmonary oxygen partial pressure evolution during apnea, Deninger *et al.*, **141**, 207 at 1.5 T, integrated head immobilization system and high-performance RF coil for, Thulborn and Shen, **139**, 26

gases: single-point ramped imaging with T_1 enhancement (SPRITE) study, Prado *et al.*, **137**, 324

gas flow, using circulating laser-polarized ¹²⁹Xe, Brunner *et al.*, **138**, 155 high-field, microimaging at 14 T using GESEPI for removal of magnetic susceptibility artifacts in T_2^* -weighted image contrast, Yang *et al.*, **141**, 1

hyperpolarized ¹²⁹Xe, implications of role of oxygenation in T_1 of ¹²⁹Xe in blood, Albert *et al.*, **140**, 264

isotropically weighted diffusion imaging, optimized pulse sequence for, Cercignani and Horsfield, **140**, 58

low-field, laser-polarized noble gas, Wong et al., 141, 217

measurement of volume magnetic susceptibility using boundary condition, Wang, Li, and Haselgrove, **140**, 477

microscopy, practical aspects of birdcage coils for, Doty et al., 138, 144 orthopedic, openable high-strength gradient set for, Crozier et al., 139, 81

self-diffusion imaging by spin echo in Earth's magnetic field, Mohorič *et al.*, **136.** 22

signal intensities in FLASH-EPI-Hybrid sequences, Hillenbrand *et al.*, **139**, 74

single-point, water adsorption in zeolite 4A pellets, Prado, Balcom, and Jama, 137, 59

single-shot line scan imaging using stimulated echoes, Finsterbusch and Frahm, 137, 144

spiral MRI gradient design, simple reliable solutions for, Salustri, Yang, and Glover, **140**, 347

triple-quantum-filtered twisted projection sodium MRI of human articular cartilage *in vivo*, Borthakur *et al.*, **141**, 286

xenon-131 surface sensitive imaging of aerogels in liquid xenon near critical point, Pavlovskaya *et al.*, **137**, 258

Magnetic resonance microscopy

¹H DNP at 1.4 T of water doped with triarylmethyl-based radical, Wind and Ardenkjær-Larsen, **141**, 347

Magnetic susceptibility

artifacts, in T_2^* -weighted image contrast, microimaging at 14 T using GESEPI for removal of, Yang *et al.*, **141**, 1

local, induced gradients, effects on water diffusion measurements in brain *in vivo*, Clark, Barker, and Tofts, **141**, 52

and origin of residual NMR linewidth of peptide bound to resin under MAS, Elbayed *et al.*, **136**, 127

volume, MRI measurement using boundary condition, Wang, Li, and Haselgrove, 140, 477

Magnetization

prepared, and centric k-space sampling, SPRITE MRI with, Mastikhin $et\ al.$, 136, 159

uncoupled, gradient $BIRD_{\scriptscriptstyle R}$ method for selecting, Heikkinen and Kilpeläinen, 137, 93

Magnetization transfer

¹⁹F 2D MAS NMR of oxyfluorides, high-order spin diffusion mechanisms in, Du, Levitt, and Grey, 140, 242

MARF imaging

enhanced by filter based on rotary echo refocusing, $T_{2\rho}$ -contrasted NMR images by, De Luca *et al.*, **139**, 126

Match conditions

Hartmann–Hahn, for CP/MAS between two half-integer quadrupolar nuclei, examples, Eastman, 139, 98

Mathematica software

SPORT-NMR package, for determination of relaxation times in unresolved NMR spectra, Geppi and Forte, **137**, 177

Matrix elements

of operator equivalents, calculation, Ryabov, 140, 141

Membrane peptides

NMR studies, lanthanide chelates as bilayer alignment tools in, Prosser *et al.*, **141**, 256

Membrane permeability

permeability coefficients from NMR *q*-space data: models with unevenly spaced semipermeable parallel membranes, Kuchel and Durrant, **139**, 258

Membranes

red blood cell, unsealed and cytoskeleton-depleted, competition between Na⁺ and Li⁺: ²³Na MQF and ⁷Li relaxation study, Srinivasan *et al.*, **140**, 206

surface analysis and localization of embedded peptides by ¹³C MAS NMR using lanthanide ions, Gröbner, Glaubitz, and Watts, **141**, 335

Meso-porous aerogels

Xenon-131 surface sensitive imaging in liquid xenon near critical point, Pavlovskaya et al., 137, 258

Metabolites

cerebral, mapping using double echo-filter metabolite imaging technique, Chen and Hu, **140**, 363

cerebral concentrations, in vivo quantitation using natural abundance 13C MRS at 1.5 T, Blüml, 136, 219

doubly and singly ¹³C-labeled, separate quantification by HSQC-filtered J spectroscopy, Davison, Jones, and Dixon, 137, 448

Metal halide complexes

halomolybdenyl, -vanadyl, and -chromyl, g values, Li et al., 138, 80 Metalloproteins

even-electron, Q-band EPR probe for quantitative studies, Petasis and Hendrich, 136, 200

Methylene groups

methylene-only subspectra in ¹³C CPMAS using double-quantum filtering sequence, Rossi, Subramanian, and Harbison, 141, 159

Methyl-α-D-glucopyranoside

pure absorption ESEEM spectra using filter-diagonalization method for harmonic inversion, Jeschke, Mandelshtam, and Shaka, 137, 221

Micromechanical detection

and electromagnetic detection, simultaneous, in EPR, Alzetta et al., 141, 148 Microscopy

high-field MRI, practical aspects of birdcage coils for, Doty et al., 138, 144 MR, ¹H DNP at 1.4 T of water doped with triarylmethyl-based radical, Wind and Ardenkjær-Larsen, 141, 347

NMR, resolution in high-field echo planar microscopy, Peters and Bowtell, **137,** 196

RF field gradient NMR, maps of self-diffusion coefficients by, Valtier, Humbert, and Canet, 141, 7

strongly coupled spin systems, spin coherence relaxation in rotating frame for, De Luca et al., 139, 126

Microwave heating

and ¹H DNP at 1.4 T of water doped with triarylmethyl-based radical, Wind and Ardenkjær-Larsen, 141, 347

Microwave limiter

cryogenically coolable, Rinard, Quine, and Eaton, 136, 207

Mixture analysis

proteins in biological buffer solutions, capillary array electrophoretic NMR, He et al., 141, 355

spectral decomposition using bilinear Bayesian approach, Ochs et al., 137,

Molecular dynamics

dual processing of 2D exchange data in MAS NMR of solids, Tycko and Berger, 141, 141

Molecular motion

measurement of longitudinal and transverse cross-correlation between ¹³C-¹H dipolar interaction and ¹³C chemical shift anisotropy, Kojima et al., 136, 169

Molecular tumbling

slow, calculation of MAS spectra influenced by, Mayer, 139, 132

Multidimensional NMR

¹³C natural abundance S³E and S³CT experiments for measurement of *J*-coupling constants between ${}^{13}C^{\alpha}$ or ${}^{1}H^{\alpha}$ and other protons in protein, Sørensen, Meissner, and Sørensen, 137, 237

high-temperature pulsed-field-gradient, of polymers, Liu et al., 140, 482 optimization of 3D HCCH TROSY-type NMR correlation of aromatic ¹H-¹³C groups in proteins, Meissner and Sørensen, **139**, 447

spin-state-selective TPPI: suppression of heteronuclear coupling constants in multidimensional NMR, Schulte-Herbrüggen et al., 139, 443

TROSY-type experiments, design of, role of coherence-transfer efficiency, Meissner and Sørensen, 139, 439

Multidimensional solid-state NMR correlation spectroscopy

experimental aspects, Ramamoorthy, Wu, and Opella, 140, 131 Multiple inversion recovery

for suppression of macromolecule resonances in short-echo-time ¹H NMR spectroscopy of human brain, Knight-Scott, 140, 228

Multiple-pulse dynamics

off-resonance, in solid-state NMR: revised coherent averaging theory analysis, Cho, 141, 164

Multiple-quantum coherence

 $HN(\alpha/\beta\text{-COCA-}J)$ experiment for measurement of ${}^{1}J_{C'C^{\alpha}}$ couplings from 2D [15N, 1H] correlation spectrum, Permi et al., 141, 44

measurement of homonuclear 2J-couplings from spin-state selective double-/zero-quantum 2D NMR spectra, Permi et al., 139, 273

and multiple spin echoes and dipolar field: significance of higher-order terms in equilibrium density matrix, Minot, Callaghan, and Kaplan, 140, 200

spin counting with fast MAS, Geen et al., 138, 167

Multiple-quantum-filtered NMR

detection of boric acid and borate ion binding to cytochrome c, Taler, Eliav, and Navon, 141, 228

¹H and ²H homonuclear and heteronuclear, dipolar interactions and dynamic processes of water in tendon, Eliav and Navon, 137, 295

²³Na, evidence for competition between Na⁺ and Li⁺ for unsealed and cytoskeleton-depleted RBC membrane, Srinivasan et al., 140, 206

triple-quantum-filtered sodium MR images of human knee joint in vivo, Borthakur et al., 141, 286

Multiple-quantum MAS

high-resolution heteronuclear correlation between quadrupolar nuclei, Chan, **140,** 487

Multiple-quantum spectroscopy

excitation in solids, selection rules, Tycko, 139, 302

HBHA(CBCACO)NH experiment, with enhanced sensitivity for partially deuterated samples, Gschwind, Kessler, and Gemmecker, 137, 285

recoupled polarization transfer heteronuclear ¹H-¹³C MQ correlation in solids under ultra-fast MAS, Saalwächter, Graf, and Spiess, 140, 471 selective correlation of amide groups to glycine alpha protons in proteins,

Bazzo, Cicero, and Barbato, 136, 15 two-dimensional, quadrupolar and chemical shift tensors characterized by,

Medek and Frydman, 138, 298

Multiple rephasing

time correlations in fluid transport obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

Multiple spin echoes

and multiple quantum coherence and dipolar field: significance of higherorder terms in equilibrium density matrix, Minot, Callaghan, and Kaplan, 140, 200

Multiplet-selective NMR

J pulses for, Bendall and Skinner, 141, 261

Multiplex probe

for simultaneous acquisition of multiple samples, Fisher et al., 138, 160 Multipolar AX spin systems

under spin locking conditions, NMR relaxation in, Kaikkonen and Kowalewski, 141, 326

Multispin order

two-spin, decorrelation, detection of intermolecular chemical exchange through, Skrynnikov and Ernst, 137, 276

Muscle

human calf, ³¹P CSI study: spectral decomposition using bilinear Bayesian approach, Ochs et al., 137, 161

MUSIC

in triple-resonance experiments: amino acid type-selective ¹H-¹⁵N correlations, Schubert et al., 141, 34

Ν

 ^{14}N

general analysis of 14 N (I = 1) ESEEM, Lee, Doan, and Hoffman, 140, 91

acetylleucine, experimental aspects of multidimensional solid-state NMR, Ramamoorthy, Wu, and Opella, 140, 131

- amino acid type-selective ¹H-¹⁵N correlations: MUSIC in triple-resonance experiments, Schubert *et al.*, **141**, 34
- barley lectin: order matrix analysis of residual dipolar couplings using singular value decomposition, Losonczi et al., 138, 334
- barstar, superslow backbone protein dynamics study by 1D solid-state MAS exchange NMR spectroscopy, Krushelnitsky et al., 138, 244
- ¹³C- and ¹⁵N-labeled octapeptide, measurement of relaxation rates of N^H and H" backbone protons, Millet et al., 139, 434
- chemical shift, of [1-¹⁵N]-2'-deoxyguanosine, magnitudes and orientations determined from polycrystalline sample by 2D solid-state NMR, Lorigan *et al.*, **140**, 315
- edited 3D-NOESY-HSQC spectra, computer-assisted assignment using back-calculated and experimental spectra, Görler et al., 137, 39
- edited 3D ROESY and NOESY HMQC and HSQC, signal enhancement using 45° water flipback for, Gruschus and Ferretti, **140**, 451
- ²H, ¹³C, ¹⁵N-labeled proteins, observation of through-hydrogen-bond ^{2h}J_{HC}, Cordier et al., **140**, 510
- ¹H–¹⁵N correlated ¹H CPMG experiments, transverse ¹H cross relaxation in, Ishima, Louis, and Torchia, **137**, 289
- ¹H¹⁵N two-spin order in L-tryptophan, decorrelation, detection of intermolecular chemical exchange through, Skrynnikov and Ernst, **137**, 276 ¹⁵N, ¹³C
 - enriched samples of transition metal complexes, measurement of magnitude and sign of heteronuclear coupling constants, Otting, Soler, and Messerle, 137, 413; erratum, 139, 186
 - magic-angle turning experiments with TPPM decoupling, resolution enhancement in, McGeorge, Alderman, and Grant, 137, 138
- ¹⁵N, ¹³C-labeled *N*-acetylglycine, 3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, **138**, 193
- ¹⁵N, ¹³C-labeled DNA oligonucleotides, thymine resonances in, HCCCH experiment for through-bond correlation of, Sklenář, Masse, and Feigon, 137, 345
- ¹⁵N, ¹³C-labeled nucleic acids and protein complexes, ³J_{H3'P} and ³J_{C4'P} in, 2D {³¹P} spin-echo-difference constant-time [¹³C, ¹H] HMQC experiment for simultaneous determination, Szyperski *et al.*, **140**, 491
- ¹⁵N, ¹³C-labeled proteins
 - BEST homonuclear adiabatic decoupling for, Zhang and Gorenstein, 138,
 - ¹³C^α-¹H^α couplings in, J^{CH}-modulated 2D (HACACO)NH pulse scheme for quantitative measurement of, Hitchens, McCallum, and Rule, 140, 281
 - measurement of ¹J_{NC'} and ²J_{HNC'} couplings from spin-state-selective 2D correlation spectrum, Permi *et al.*, **140**, 32
 - selective correlation of amide groups to glycine alpha protons by multiple quantum spectroscopy, Bazzo, Cicero, and Barbato, **136**, 15
- ¹⁵N, ¹³C-labeled RNA, triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in, Wöhnert et al., 139, 430
- ¹⁵N-coupled protons, in vivo detection in rat brain by ISIS localization and multiple-quantum editing, Kanamori and Ross, 139, 240
- ¹⁵N-²H distance measurements, applications of deuterium REDOR, Sack et al., 138, 54
- ¹⁵N-labeled photoactive yellow protein, photointermediates, NMR experiments, Rubinstenn et al., 137, 443
- 15N-labeled proteins
 - ^{3}J (H $_{\rm N}$ H $_{\rm a}$) couplings in, *J*-multiplied HSQC method for measurement of, Heikkinen *et al.*, **137**, 243
 - TROSY-type ¹H NMR NOESY spectra, suppression of diagonal peaks, Meissner and Sørensen, **140**, 499
- 15N-labeled ubiquitin
 - identification of spin diffusion pathways in, Eykyn, Früh, and Bodenhausen, 138, 330
 - measurement of relaxation rates of N^H and H^α backbone protons, Millet et al., 139, 434

- NMR, excitation of selected proton signals in, Pelupessy, Chiarparin, and Bodenhausen, **138**, 178
- off-resonance ROESY, tilt angle dependence of cross-relaxation in, Cutting, Ghose, and Bodenhausen, 138, 326
- offset profiles of selective pulses in, Eykyn, Ghose, and Bodenhausen, 136, 211
- uniformly labeled, ¹³C selectively labeled, determination of multiple φ-torsion angles by 2D solid-state NMR, Hong, **139**, 389
- one-bond ¹⁵N-¹H coupling constants in protein backbone, pulse sequences for measurement, Lerche *et al.*, **140**, 259
- REDOR-determined distances from heterospins to clusters of ¹³C labels, Schaefer, **137**, 272
- triosephosphate isomerase, TROSY: sensitivity improvement, Rance, Loria, and Palmer, 136, 92
- 2D [15 N, 1 H] correlation spectrum, HN(α/β -COCA-J) experiment for measurement of $^{1}J_{C'C^{\alpha}}$ couplings from, Permi *et al.*, **141**, 44
- ubiquitin, measurement of homonuclear ²*J*-couplings from spin-state selective double-/zero-quantum 2D NMR spectra, Permi *et al.*, **139**, 273
- yeast triose-phosphate isomerase, TROSY gradient-enhanced triple-resonance NMR spectroscopy, Loria, Rance, and Palmer, 141, 180

Na+

and Li⁺, competition for unsealed and cytoskeleton-depleted human RBC membrane: ²³Na MQF and ⁷Li relaxation study, Srinivasan *et al.*, **140**, 206

²³Na

- multiple-quantum-filtered NMR evidence for competition between Na⁺ and Li⁺ for unsealed and cytoskeleton-depleted RBC membrane, Srinivasan *et al.*, **140**, 206
- Na₂B₄O₇, Hartmann–Hahn match conditions for CP/MAS between two half-integer quadrupolar nuclei, Eastman, **139**, 98
- NMR spectra, of sodium ions in ordered environments in biological systems, analysis, Kemp-Harper, Wickstead, and Wimperis, **140**, 351

 $Na_2B_4O_7$

²³Na, Hartmann-Hahn match conditions for CP/MAS between two halfinteger quadrupolar nuclei, Eastman, 139, 98

Narrowband excitation

²H powder pattern, and application to ²H 1D exchange sample-turning NMR, Reichert et al., 139, 308

Neural networks

permeability coefficients from NMR *q*-space data: models with unevenly spaced semipermeable parallel membranes, Kuchel and Durrant, **139**, 258

Neuronal activity

current-induced magnetic resonance phase imaging, Bodurka *et al.*, **137**, 265 NH groups

selection, asymmetric adiabatic pulses, Hwang, van Zijl, and Garwood, 138, 173

Nitroxide

side-chain dynamics, in spin-labeled helix-forming peptide, by high-frequency EPR, Bennati *et al.*, **139**, 281

NMR

application of Berry's phase in presence of non-adiabatic environment, Gaitan, 139, 152

error-tolerant Litz RF coils, Doty, Entzminger, and Hauck, 140, 17

- log data sets with different measurement errors, inversion of, Dunn and LaTorraca, 140, 153
- q-space experiments, estimation of permeability coefficients from, Kuchel and Durrant, 139, 258

NMR flow imaging

fast, in plants, using FLASH imaging, Rokitta, Zimmermann, and Haase, 137, 29

NMR imaging

magic echo solid-state, without rapidly switchable field gradient, Matsui *et al.*, **138**, 220

relaxation, selective imaging of biofilms in porous media by, Hoskins et al.,

thermally polarized helium-3 gas, Kober et al., 138, 308

NMR microscopy

resolution in high-field echo planar microscopy, Peters and Bowtell, 137,

RF field gradient, maps of self-diffusion coefficients by, Valtier, Humbert, and Canet, 141, 7

NMR probes

for simultaneous acquisition of multiple samples, Fisher et al., 138, 160 NMR q-space plots

coherence features in, assignment to particular diffusion modes in RBC suspensions, Torres et al., 138, 135

NMR quantum logic gates

construction and implementation for two-spin systems, Price et al., 140, 371 NMR spectra

¹H, of human skeletal muscle, creatine resonances in, effect of exercise, Kreis et al., 137, 350

normalization, algorithm for, Romano et al., 138, 115

rotating solids, efficient spectral simulations: γ -COMPUTE, Hohwy et al.,

spectral fitting using alternating optimization method with a priori knowledge, Bi et al., 140, 108

NMR spectroscopy

¹H, human brain, suppression of macromolecule resonances at short echo times, application of multiple inversion recovery, Knight-Scott, 140,

mapping brain metabolites using double echo-filter metabolite imaging technique, Chen and Hu, 140, 363

natural abundance 13C, at 1.5 T, in vivo quantitation of cerebral metabolite concentrations using, Blüml, 136, 219

from proton spin magnetization in rotating frame: study of small tunneling splitting, Damyanovich, Peternelj, and Pintar, 140, 9

selective injection of magnetization by slow chemical exchange, Boulat, Epstein, and Rance, 138, 268

series of biomedical MRS signals, time-domain quantification, Vanhamme et al., 140, 120

NMR theory

derivation of selection rules for multiple-quantum NMR excitation in solids, Tycko, 139, 302

NOAH

self-correcting distance gemometry-based program, automated 2D NOESY assignment and structure calculation of crambin with, Xu et al., 136, 76

chemical exchange-relayed, in NMR experiments for observation of protein-water interactions, editing, Melacini, Kaptein, and Boelens, 136, 214

consequences of 129Xe-1H cross relaxation in aqueous solutions, Stith et al., 139, 225

and ¹H DNP at 1.4 T of water doped with triarylmethyl-based radical, Wind and Ardenkjær-Larsen, 141, 347

long-range nuclear Overhauser enhancement, quantitative measurement, Harris et al., 140, 504

long-range small-molecule, observation using sensitivity enhancement scheme, Van, Smith, and Shaka, 141, 191

¹⁷O-{ ¹H} NOE in water, isotope effects, Sergeyev, Sergeyeva, and Raynes,

selective, identification of spin diffusion pathways in isotopically labeled biomolecules, Eykyn, Früh, and Bodenhausen, 138, 330

NOESY

automated 2D, assignment and structure calculation of crambin with selfcorrecting distance geometry-based NOAH/DIAMOD programs, Xu et al., 136, 76

high-resolution HMQC-NOESY-HSQC spectroscopy, Morshauser and Zuiderweg, 139, 232

¹H NMR TROSY-type spectra of ¹⁵N-labeled proteins, suppression of diagonal peaks, Meissner and Sørensen, 140, 499

2D unbiased, and 1D techniques, comparison for measurement of CSA/DD cross-correlated relaxation, Batta, Kövér, and Kowalewski, 136, 37

NOESY-HMOC

3D ¹⁵N-edited, signal enhancement using 45° water flipback, Gruschus and Ferretti, 140, 451

NOESY-HSQC

3D ¹⁵N-edited, signal enhancement using 45° water flipback, Gruschus and Ferretti, 140, 451

NOESY-NOESY

protein hydration study using slaved pulses, Bornet, Guerlesquin, and Piotto, **138,** 107

NOESY-TOCSY

protein hydration study using slaved pulses, Bornet, Guerlesquin, and Piotto, 138, 107

Noise (see also Signal-to-noise ratio)

EPR, absolute intensity, Rinard et al., 140, 69

 t_1 , incoherent, conversion of coherent artifacts into: randomized acquisition for suppression of artifacts in 2D NMR, Bowyer, Swanson, and Morris, **140,** 513

Non-adiabatic environment

Berry's phase in presence of, with application to magnetic resonance, Gaitan, 139, 152

Nonideal gradients

 B_1 field distribution with, mapping in high-resolution NMR spectrometer, Jerschow and Bodenhausen, 137, 108

Nonionic surfactants

clays suspended in aqueous solutions of, ⁷Li double-quantum filtered NMR and multinuclear relaxation rates, Grandjean and Robert, 138, 43

Non-Kramers doublet

ENDOR and ESEEM study, S = 2 ferrous ion of $[Fe(II)EDTA]^{2-}$, Song et al., 141, 291

Nonlinear least squares

for parameter estimation for accurate quantification of ¹H spectra, Sundin et al., 139, 189

in time-domain quantification of series of biomedical MR spectroscopy signals, Vanhamme et al., 140, 120

Normalization

NMR spectra, algorithm for, Romano et al., 138, 115

Nuclear magnetic relaxation dispersion

high-resolution, measurements of solute spin probes, using dual-magnet system, Wagner et al., 140, 172

Nuclear Overhauser effect (see NOE)

Nuclear Overhauser effect spectroscopy (see NOESY)

Nuclear Overhauser enhancement

long-range, quantitative measurement of, Harris et al., 140, 504

Nuclear parameters

large-magnitude high-spin, in Ti³⁺ center, from X-band EPR measurements at 10 K, Tennant and Claridge, 137, 122

Nuclear quadrupole resonance

SORC pulse sequence

feedback optimization of offset frequency, Blauch, Schiano, and Ginsberg, 139, 139

feedback optimization of pulse width, Schiano et al., 140, 84

spins $\frac{3}{2}$, calculations of multipulse sequence in, Odin, 141, 239

Nuclear quadrupole resonance imaging

phase-modulated rotating frame techniques, for spatial encoding, Casanova, Robert, and Pusiol, 141, 62

powder, image reconstruction with real gradient coils, Swaminathan and Suits, 138, 123

Nucleic acids

13C-labeled

³J(H3'_i, P_{i+1}) and ³J(H5'_i/5"_i, P_i) coupling constants in, determination using CT-HMQC, Hu et al., 139, 181

³J_{H3'P} and ³J_{C4'P} in, 2D {³¹P} spin-echo-difference constant-time [¹³C, ¹H] HMQC experiment for simultaneous determination, Szyperski *et al.*, **140**, 491

Numerical diagonalization

spin Hamiltonian, modeling EPR powder spectra using, Morin and Bonnin, 136, 176

Numerical method

lineshape calculations on spreadsheet software, Mayer, 138, 1

Numerical optimization

magic-angle spinning NMR spectroscopy with composite pulses, Leppert, Heise, and Ramachandran, 139, 382

Numerical simulation

analysis of *J* coupling-induced fat suppression in DIET imaging, Stables *et al.*, **136**, 143

density matrix, of effects of *J* coupling in spin-echo and fast spin-echo imaging, Stables *et al.*, **140**, 305

Nutation spectra

calculations of multipulse sequence in NQR of spins $\frac{3}{2}$, Odin, 141, 239

0

Obituary

Regitze R. Vold, 138, v

Octapeptide

¹³C- and ¹⁵N-labeled, measurement of relaxation rates of N^H and H^a back-bone protons, Millet *et al.*, **139**, 434

Off-magic-angle spinning

as tool for analysis of slow tumbling motions, Mayer, 139, 132

Off-resonance ROESY (off-resonance rotating-frame Overhauser effect spectroscopy)

longitudinal and transverse cross-relaxation rates from, quantitative measurement, Malliavin *et al.*, **140**, 189

tilt angle dependence of cross-relaxation in, Cutting, Ghose, and Bodenhausen, 138, 326

Off-resonance synchronization

ORSAT and modifications of SEFT and APT, Beckmann, Dietrich, and Radeglia, 137, 132

Offset frequency

in SORC pulse sequence, optimization using feedback, Blauch, Schiano, and Ginsberg, **139**, 139

Offset-independent adiabaticity

evolution strategy optimization for adiabatic pulses in MRI, Lunati *et al.*, **138**, 48

Offset profiles

selective pulses in isotopically labeled macromolecules, Eykyn, Ghose, and Bodenhausen, ${\bf 136},\,211$

¹⁷O, ¹H coupling constant

in water, isotope effects, Sergeyev, Sergeyeva, and Raynes, 137, 311 Oligonucleotides

DNA, ¹³C-labeled, thymine resonances in, HCCCH experiment for throughbond correlation of, Sklenář, Masse, and Feigon, **137**, 345

One-dimensional NMR

and 2D unbiased experiments, comparison for measurement of CSA/DD cross-correlated relaxation, Batta, Kövér, and Kowalewski, **136**, 37

isotopically labeled macromolecules, excitation of selected proton signals in, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

solid-state MAS exchange NMR, superslow backbone protein dynamics study, Krushelnitsky et al., 138, 244

spectra, simulations, pulsed-field gradients in, Meresi et al., 137, 186 Operator equivalents

generation, and calculation of matrix elements, Ryabov, 140, 141

Optimization

diffusion tensor imaging using MRI, Papadakis *et al.*, **137**, 67 evolution strategy, for adiabatic pulses in MRI, Lunati *et al.*, **138**, 48 fast, of biplanar gradient coil set, Tomasi *et al.*, **140**, 325

feedback, of pulse width in SORC sequence, Schiano *et al.*, **140**, 84 high-resolution HMQC–NOESY–HSQC spectroscopy, Morshauser and Zuiderweg, **139**, 232

numerical, MAS NMR spectroscopy with composite pulses, Leppert, Heise, and Ramachandran, 139, 382

offset frequency in SORC pulse sequence, using feedback, Blauch, Schiano, and Ginsberg, 139, 139

pulse sequence for isotropically weighted diffusion imaging, Cercignani and Horsfield, **140**, 58

Orbitally nondegenerate state

g-matrix based on configuration interaction and Stone's perturbation theory, Li et al., 138, 74

Ordered environments

in biological systems, sodium ions in, analysis of ²³Na NMR spectra, Kemp-Harper, Wickstead, and Wimperis, **140**, 351

Order matrix analysis

residual dipolar couplings, using singular value decomposition, Losonczi *et al.*, **138**, 334

Organic solids

dynamic nuclear polarization in pulsed ENDOR, Kouskov et al., 137, 25 Orientation

anisotropic, lactate in skeletal muscle, observed by dipolar coupling in ¹H NMR spectroscopy, Asllani *et al.*, **139**, 213

Orientational constraints

¹³C selective polarization and spin diffusion in lipid bilayer-bound polypeptide by solid-state NMR, Tian, Fu, and Cross, 139, 377

Oriented model membrane

lanthanide chelates as bilayer alignment tools in NMR studies of membrane peptides, Prosser *et al.*, **141**, 256

Oriented systems

and static systems, multipulse solid-state NMR on, structural parameters from ¹⁹F homonuclear dipolar couplings by, Grage and Ulrich, **138**, 98

ORSAT

and modifications of SEFT and APT, in $^{13}{\rm C}$ signal assignment, Beckmann, Dietrich, and Radeglia, 137, 132

Orthopedic MRI

openable high-strength gradient set for, Crozier *et al.*, **139**, 81

¹⁹F NMR, high-order spin diffusion mechanisms in, Du, Levitt, and Grey, 140, 242

Oxygenation

role in T_1 of ¹²⁹Xe in blood, Albert *et al.*, **140**, 264

Oxygen partial pressure

regional intrapulmonary, evolution during apnea, quantification by ³He MRI, Deninger *et al.*, **141**, 207

Ρ

 $^{31}\mathbf{P}$

CSI studies of human head and calf muscle: spectral decomposition using bilinear Bayesian approach, Ochs et al., 137, 161

³*J*(H3'_i, P_{i+1}) and ³*J*(H5'/5", P_i) coupling constants, determination in ¹³C-labeled nucleic acids using CT-HMQC, Hu *et al.*, **139**, 181

2D $\{^{31}P\}$ spin-echo-difference constant-time $[^{13}C, ^{1}H]$ HMQC experiment for simultaneous determination of $^{3}J_{H3:P}$ and $^{3}J_{C4:P}$ in ^{13}C -labeled nucleic acids and protein complexes, Szyperski *et al.*, **140**, 491

Parallel detection

NMR probe for simultaneous acquisition of multiple samples, Fisher $\it et~al., 138, 160$

Parallel planes

unevenly spaced semipermeable membranes, models, estimation of permeability coefficients from q-space experiments, Kuchel and Durrant, 139,

Paramagnetic effects

on nuclear relaxation in enzyme-bound Co(II)-adenine nucleotide complexes, role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

Paramagnetic ions

lanthanide, 13C MAS using, probing membrane surfaces and location of membrane-embedded peptides with, Gröbner, Glaubitz, and Watts, **141,** 335

Paramagnetic relaxation enhancement

low-symmetry complexes for electron spin quantum number $S = \frac{5}{2}$, generalized MSBM theory, Strandberg and Westlund, 137, 333

Partial-data transform

transforming NMR data despite missing points, Kuethe et al., 139, 18

PASS shifted echo: chemical bonding of lead through isotropic vs anisotropic correlation, Fayon et al., 137, 116

²⁰⁷Ph

chemical bonding of lead in glasses through isotropic vs anisotropic correlation: PASS shifted echo, Fayon et al., 137, 116

Pentacene

in p-terphenyl crystals, triplet state, dynamic nuclear polarization in pulsed ENDOR, Kouskov et al., 137, 25

NMR microscopy using, resolution, Peters and Bowtell, 137, 196

backbone and side chain sites, application of 2D and 3D ¹H/¹³C PISEMA experiments, Gu and Opella, 140, 340

bound to resin under MAS, origin of residual NMR linewidth of, Elbayed et al., 136, 127

¹³C- and ¹⁵N-labeled, 3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, 138, 193

helix-forming, spin-labeled, nitroxide side-chain dynamics by high-frequency EPR, Bennati et al., 139, 281

membrane-embedded, localization by 13C MAS NMR using lanthanide ions, Gröbner, Glaubitz, and Watts, 141, 335

Perdeuterated proteins

¹H-¹⁵N correlated ¹H CPMG experiments, transverse ¹H cross relaxation in, Ishima, Louis, and Torchia, 137, 289

observation of through-hydrogen-bond ^{2h}J_{HC}, Cordier et al., **140**, 510 Phase adjustment of spinning sidebands (see PASS)

Phase contrast

fast-DENSE high-resolution strain analysis of human heart, Aletras, Balaban, and Wen, 140, 41

Phase correction

zero-order, in ¹H NMR, introduced artifacts and method of elimination by phase filtering, Wild, 137, 430

Phase filtering

elimination of artifacts introduced by zero-order phase correction in ¹H NMR, Wild, 137, 430

Phase imaging

current-induced MRI, Bodurka et al., 137, 265

Phase modulation

rotating-frame NQR techniques for spatial encoding using, Casanova, Robert, and Pusiol, 141, 62

Phase-sensitive 2D NMR spectra

composite PFGs with refocused chemical shifts and short recovery time, Hu and Shaka, 136, 54

resolution enhancement in 13C and 15N magic-angle turning with TPPM decoupling, McGeorge, Alderman, and Grant, 137, 138

Photoactive yellow protein

photointermediates, NMR experiments, Rubinstenn et al., 137, 443 Photointermediates

NMR experiments: photoactive yellow protein, Rubinstenn et al., 137, 443 **PISEMA**

experimental aspects of multidimensional solid-state NMR correlation spectroscopy, Ramamoorthy, Wu, and Opella, 140, 131

two-dimensional NMR of [1-15N]-2'-deoxyguanosine polycrystalline sample, magnitudes and orientations of 15N chemical shift, Lorigan et al., 140, 315

two- and three-dimensional ¹H/¹³C experiments and application to backbone and side chain sites of amino acids and peptides, Gu and Opella, 140,

Plants

fast NMR flow measurements using FLASH imaging, Rokitta, Zimmermann, and Haase, 137, 29

Polarization transfer

analytical transfer functions for four coupled spins $\frac{1}{2}$ under isotropic mixing conditions, Luy, Schedletzky, and Glaser, 138, 19

Polycrystalline sample

[1-15N]-2'-deoxyguanosine, magnitudes and orientations of 15N chemical shift determined by 2D solid-state NMR, Lorigan et al., 140, 315

EPR spectrum, evaluation of spin-Hamilltonian parameters and linewidth from, Misra, 140, 179

Polyethylene

high-temperature pulsed-field-gradient multidimensional NMR, Liu et al., **140,** 482

Poly(ethylene glycol) monoalkyl ethers

clays suspended in aqueous solutions of, ⁷Li double-quantum filtered NMR and multinuclear relaxation rates, Grandjean and Robert, 138, 43

Polyglycine

superslow backbone protein dynamics study by 1D solid-state MAS exchange NMR spectroscopy, Krushelnitsky et al., 138, 244

fluorinated, cross-polarization dynamics between ¹⁹F and ¹H, analysis based on spin thermodynamics theory, Ando, Harris, and Reinsberg, 141, 91

high-temperature pulsed-field-gradient multidimensional NMR, Liu et al., **140,** 482

semicrystalline, solid-state wideline heteronuclear correlation experiments: isotropic mixing, sign discrimination, and sensitivity, Oliver and Titman, 140, 235

solid, T₂₀-contrasted NMR images, De Luca et al., 139, 126

Polypeptides

helical, ¹³C-labeled, numerical simulations of MQ NMR signal amplitudes and experimental MQ excitation spectra, Tycko, 139, 302

lipid bilayer-bound, 13C selective polarization and spin diffusion by solidstate NMR, Tian, Fu, and Cross, 139, 377

Porous media

biofilms in, selective imaging by NMR relaxation, Hoskins et al., 139, 67 echo-planar imaging with spatial resolution below 100 µm, Manz, Chow, and Gladden, 136, 226

fluid transport in, time correlations obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

planar, cylindrical, and spherical pores with wall relaxivity, spin echo analysis of restricted diffusion under generalized gradient waveforms, Codd and Callaghan, 137, 358

Powder

EPR spectra

modeling using numerical diagonalization of spin Hamiltonian, Morin and Bonnin, 136, 176

simulation, Misra, 137, 83

NQR images, reconstruction with real gradient coils, Swaminathan and Suits, 138, 123

simulation of MR static powder lineshapes, Ponti, 138, 288

Powder average

calculations of multipulse sequence in NQR of spins $\frac{3}{2}$, Odin, 141, 239 Power reduction

evolution strategy optimization for adiabatic pulses in MRI, Lunati *et al.*, **138.** 48

PRAWN

mixing sequences for selective heteronuclear *J* cross polarization, Chandrakumar and Kimmich, **137**, 100

Prepared magnetization

and centric *k*-space sampling, SPRITE MRI with, Mastikhin *et al.*, **136**, 159 *a Priori* knowledge

alternating optimization method with, spectral fitting of NMR spectra using, Bi et al., 140, 108

Probes

NMR (see NMR probes)

Product operator formalism

spectral simulations incorporating gradient coherence selection, Young et al., 140, 146

Product operators

exact product operator evolution of weakly coupled spin- $\frac{1}{2}$ I_mS_n systems during arbitrary RF irradiation of I spins, Skinner and Bendall, **141**, 271 *J* pulses for multiplet-selective NMR, Bendall and Skinner, **141**, 261

Propagators

two-dimensional, time correlations in fluid transport obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

Protein dynamics

superslow backbone protein dynamics with 1D solid-state MAS exchange NMR spectroscopy, Krushelnitsky et al., 138, 244

tilt angle dependence of cross-relaxation in off-resonance ROESY, Cutting, Ghose, and Bodenhausen, 138, 326

Protein hydration

evaluation of slaved pulses for study of, Bornet, Guerlesquin, and Piotto, 138, 107

Protein NMR

isotopically labeled biomolecules

identification of spin diffusion pathways, Eykyn, Früh, and Bodenhausen, 138, 330

offset profiles of selective pulses, Eykyn, Ghose, and Bodenhausen, **136**, 211

selective excitation of proton signals, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

sensitivity-enhanced sim-CT HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH triple-resonance experiments, Swapna and Montelione, 137, 437

Protein-nucleic acid complexes

with ¹³C-labeled nucleic acids, ³J_{H3'P} and ³J_{C4'P} in, 2D {³¹P} spin-echodifference constant-time [¹³C, ¹H] HMQC experiment for simultaneous determination, Szyperski *et al.*, **140**, 491

Proteins

amino acid type-selective ¹H-¹⁵N correlations: MUSIC in triple-resonance experiments, Schubert *et al.*, **141**, 34

aromatic ¹H-¹³C groups, optimization of 3D HCCH TROSY-type NMR correlation of, Meissner and Sørensen, **139**, 447

backbone, one-bond ¹⁵N-¹H coupling constants in, pulse sequences for measurement, Lerche *et al.*, **140**, 259

in biological buffer solutions, capillary array electrophoretic NMR, He *et al.*, **141**, 355

¹³C^α or ¹H^α and other protons in, measurement of *J*-coupling constants between, ¹³C natural abundance S³E and S³CT experiments for, Sørensen, Meissner, and Sørensen, 137, 237

distance measurements in solid-state NMR, practical methods: constant-time rotational resonance, Balazs and Thompson, 139, 371

high-resolution HMQC-NOESY-HSQC spectroscopy, Morshauser and Zuiderweg, 139, 232

 $\mathrm{H^N-H^\alpha}$ residual dipolar couplings in, measurement, Cai *et al.*, **139**, 451 labeled (*see specific label*)

multiple ϕ -torsion angles in, determination by selective and extensive ¹³C labeling and 2D solid-state NMR, Hong, **139**, 389

selective correlation of amide groups to glycine alpha protons and arginine guanidine groups to delta protons by multiple quantum spectroscopy, Bazzo, Cicero, and Barbato, 136, 15

spectra assignment, amino acid type-selective triple-resonance experiments: ¹H-¹⁵N correlations, Schubert *et al.*, **141**, 34

structure determination, application of 2D and 3D $^{1}H/^{13}C$ PISEMA experiments, Gu and Opella, **140**, 340

Protein-water interactions

editing of chemical exchange-relayed NOEs in NMR experiments for observation of, Melacini, Kaptein, and Boelens, 136, 214

Proton exchange

effect on measurement of dipolar interactions in water molecules in tendon,

¹H and ²H homonuclear and heteronuclear MQF NMR study, Eliav and
Navon, **137**, 295

Proton homonuclear dipolar decoupling

methods, in ¹³C NMR of liquid crystals, Fung, Ermolaev, and Yu, **138**, 28 Proton NMR

brain

short-echo-time NMR spectra, in vivo quantification of 18 metabolites (rat), Pfeuffer et al., 141, 104

suppression of macromolecule resonances at short echo times using multiple inversion recovery (human), Knight-Scott, **140**, 228

imaging of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, **140**, 432

low-frequency, external unit for analysis of large foodstuff samples, Capozzi et al., 138, 277

selective injection of magnetization by slow chemical exchange, Boulat, Epstein, and Rance, 138, 268

skeletal muscle

anisotropic orientation of lactate observed by dipolar coupling in (bovine, rat), Asllani *et al.*, **139**, 213

creatine resonances in spectra, effect of exercise (human), Kreis *et al.*, **137**, 350

zero-order phase correction in, introduced artifacts and method of elimination by phase filtering, Wild, ${\bf 137,}~430$

Protons

 $^{1}H^{\alpha}$

in glycine, selective correlation of amide groups in proteins to, by multiple-quantum spectroscopy, Bazzo, Cicero, and Barbato, **136**, 15

and other protons in protein, and ¹³C^α, measurement of *J*-coupling constants between, ¹³C natural abundance S³E and S³CT experiments for, Sørensen, Meissner, and Sørensen, 137, 237

high-resolution magnetic relaxation dispersion measurements using dualmagnet system, Wagner et al., 140, 172

 $^{3}J(\text{H3}'_{i}, P_{i+1})$ and $^{3}J(\text{H5}'_{i}/5''_{i}, P_{i})$ coupling constants, determination in $^{13}\text{C-labeled}$ nucleic acids using CT-HMQC, Hu *et al.*, **139**, 181

¹⁵N-coupled, in vivo detection in rat brain by ISIS localization and multiplequantum editing, Kanamori and Ross, 139, 240

 $N^{\rm H}$ and H^{α} backbone protons in proteins, measurement of relaxation rates, Millet *et al.*, **139**, 434

Proton side-chain assignment

multi-quantum HBHA(CBCACO)NH experiment, with partially deuterated samples, Gschwind, Kessler, and Gemmecker, 137, 285

Proton signals

selective excitation, in NMR of isotopically labeled macromolecules, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

Proton spectra

accurate quantification: finite impulse response filter design for solvent suppression and parameter estimation, Sundin *et al.*, **139**, 189

Proton spin magnetization

in rotating frame, spectroscopy from: study of small tunneling splitting, Damyanovich, Peterneli, and Pintar, **140**, 9

Pulsed ENDOR

dynamic nuclear polarization in, Kouskov et al., 137, 25

at 140 GHz, Bennati et al., 138, 232

W-band, spectrometer for, setup and application to transition metal centers, Gromov et al., 139, 8

Pulsed EPR

dead time-dependent line distortions in absolute ESEEM spectra, Van Doorslaer, Sierra, and Schweiger, 136, 152

general analysis of 14 N (I=1) ESEEM, Lee, Doan, and Hoffman, **140**, 91 low-field pulsed dynamic nuclear polarization, Alecci and Lurie, **138**, 313 Pulsed-field gradients

composite, with refocused chemical shifts and short recovery time, Hu and Shaka, 136, 54

high-temperature multidimensional NMR of polymers, Liu *et al.*, **140**, 482 large gradient pulses, associated artifactual attenuation in PGSE NMR diffusion measurements, diagnosing and alleviating, Price *et al.*, **139**, 205

 ω_1 -filtered TOCSY with, Xu, Zhang, and Evans, 138, 127

one-dimensional double PFG spin-echo NOE, sensitivity enhancement, Van, Smith, and Shaka, **141**, 191

sequential rephasing, time correlations in fluid transport obtained by, Stapf, Damion, and Packer, 137, 316

in signal enhancement using 45° water flipback for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

signal selection in high-resolution NMR

design of gradient pulse sequences, Thomas *et al.*, **137**, 10 geometrical analysis, Mitschang, **137**, 1

in simulations of 1D and 2D NMR spectra, Meresi et al., 137, 186

unwanted signal leakage in excitation sculpting with single axis gradients, Jerschow, 137, 206

Pulsed-field gradient spin echo

and excitation sculpting, band-selective HSQC and HMBC experiments using, Gaillet et al., 139, 454

method for diffusion measurements in presence of internal gradients, Sørland, Aksnes, and Gjerdåker, 137, 397

Pulsed-gradient spin-echo NMR

diffusion measurements, artifactual attenuation associated with large gradient pulses, diagnosing and alleviating, Price et al., 139, 205

theory of spin echo in restricted geometries under stepwise gradient pulse sequence, Barzykin, **139**, 342

Pulse parameter optimization

feedback optimization of pulse width in SORC sequence, Schiano et al., 140, 84

Pulse sequence

density matrix simulations of effects of J coupling in spin-echo and fast spin-echo imaging, Stables et al., 140, 305

DIET, imaging using, J coupling-induced fat suppression in, Stables *et al.*, 136, 143

gradient, design: signal selection in high-resolution NMR by pulsed-field gradients, Thomas *et al.*, **137**, 10

for measurement of one-bond ¹⁵N-¹H coupling constants in protein backbone, Lerche *et al.*, **140**, 259

optimized, for isotropically weighted diffusion imaging, Cercignani and Horsfield, **140**, 58

stimulated anti-echo selection in spatially localized NMR spectroscopy, Zhu and Smith, 136, 1

2D (HACACO)NH, J^{CH} -modulated, for quantitative measurement of $^{13}C^{\alpha}$ – $^{1}H^{\alpha}$ couplings in ^{15}N , ^{13}C -labeled proteins, Hitchens, McCallum, and Rule, **140**, 281

Pure-phase spectra

without unwanted cross peaks: 2D exchange NMR spectra under slow MAS, Ernst, Kentgens, and Meier, 138, 66

Pyrimidine

triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in ¹³C, ¹⁵N-labeled RNA, Wöhnert et al., **139**, 430

Q

Q-band EPR probe

for quantitative studies of even-electron metalloproteins, Petasis and Hendrich, 136, 200

OPASS

multiple-rotor-cycle pulse sequences: sideband separation with ¹³⁹La NMR application, Aurentz *et al.*, **138**, 320

a-spac

permeability coefficients from NMR q-space data: models with unevenly spaced semipermeable parallel membranes, Kuchel and Durrant, 139, 258

q-space plots

coherence features in, assignment to particular diffusion modes in erythrocyte suspensions, Torres et al., 138, 135

Quadrupolar interactions

⁷Li double-quantum filtered NMR of clay suspensions, Grandjean and Robert, **138**, 43

multiple-rotor-cycle QPASS pulse sequences: sideband separation with ¹³⁹La NMR application, Aurentz *et al.*, **138**, 320

Quadrupolar nuclei

half-integer

CP/MAS between, examples of Hartmann–Hahn match conditions for, Eastman, 139, 98

shift tensors characterized by 2D multiple-quantum NMR spectroscopy, Medek and Frydman, 138, 298

high-resolution heteronuclear correlation between, Chan, 140, 487

in liquids, line narrowing of $I = \frac{1}{2}$ spins coupled to, effects of weak decoupling fields, Bendel and Baram, **141**, 121

Quadrupolar relaxation

cross-related, and carbon-13 lineshapes in $^{13}\text{CD}_2$ spin grouping, Werbelow et al., 140, 1

in system of spin- $\!\frac{1}{2}$ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali, 136, 27

Quantum computation

efficient refocusing of one-spin and two-spin interactions for, Jones and Knill, 141, 322

Quantum logic gates

NMR, construction and implementation for two-spin systems, Price et al., 140, 371

QUIET-BIRD-NOESY

attenuation of cross-peak intensities, Cutting and Bodenhausen, 140, 289

R

Radiation damping

in low-field imaging of laser-polarized noble gas, Wong *et al.*, **141**, 217 Radiation damping suppression

in high-resolution NMR, Barjat, Mattiello, and Freeman, **136**, 114 signal enhancement using 45° water flipback for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

Radiofrequency

arbitrary RF irradiation of I spins, exact product operator evolution of weakly coupled spin- $\frac{1}{2}$ I_mS_n systems during, Skinner and Bendall, **141**, 271

arbitrary RF irradiation of one spin, exact product operator evolution of weakly coupled spin- $\frac{1}{2}$ I_mS_n systems during: J pulses, Bendall and Skinner, 141, 261

transient MR without RF field pulses: fast field switching, Sloop, Lin, and Ackerman, 139, 60

Radiofrequency coils

error-tolerant Litz coils for NMR/MRI, Doty, Entzminger, and Hauck, 140,

Radiofrequency-driven dipolar recoupling

¹³C distance measurements in p-xylene/Dianin's inclusion compound by, Zaborowski, Zimmermann, and Vega, 136, 47

Radiofrequency field gradient NMR microscopy

maps of self-diffusion coefficients by, Valtier, Humbert, and Canet, 141, 7 Radiofrequency field gradients

nuclear longitudinal relaxation time images by, Humbert *et al.*, **138**, 164 Radiofrequency field homogeneity

method for determining B_1 field inhomogeneity: bias estimation in heteronuclear relaxation experiments, Guenneugues, Berthault, and Desvaux, 136. 118

Radiofrequency homogeneity

methods for characterizing a decoupler channel using undetectable quantum coherences, Bendall and Skinner, 139, 175

Radiofrequency pulse design

application of near-resonance solution to Bloch equations, Xu and Chan, ${\bf 138}, 225$

Radiofrequency pulse trains

velocity selective, Norris and Schwarzbauer, 137, 231

Radiofrequency time-domain EPR spectroscopy/imaging

high-speed data acquisition system and receiver configurations, Subramanian et al., 137, 379

Ranalexin

internal dynamics in water and TFE: quantitative measurement of longitudinal and transverse cross-relaxation rates, Malliavin *et al.*, **140**, 189

Randomized acquisition

for suppression of systematic F_1 artifacts in 2D NMR, Bowyer, Swanson, and Morris, **140**, 513

Rapid pulsing artifacts

in 2D NMR, randomized acquisition for suppression of, Bowyer, Swanson, and Morris, **140**, 513

Rapid scan stopped flow EPR

dielectric resonator-based, Sienkiewicz et al., 136, 137

RARE

knee images using openable high-strength gradient set, Crozier et al., 139, 81

87Rb

salts, shift tensors characterized by 2D multiple-quantum NMR spectroscopy, Medek and Frydman, 138, 298

spin diffusion, in ferroelectric RbH_2PO_4 studied by 2D exchange NMR, Cereghetti and Kind, 138, 12

RbH₂PO

ferroelectric, ⁸⁷Rb spin diffusion studied by 2D exchange NMR, Cereghetti and Kind, **138**, 12

Recoupling methods

recoupled polarization transfer heteronuclear ¹H-¹³C multiple-quantum correlation in solids under ultra-fast MAS, Saalwächter, Graf, and Spiess, **140**, 471

Recoupling sequence

C7, spin counting with fast MAS based on, Geen et al., 138, 167 REDOR

¹³C-²⁷Al, for detection of ¹³C-²⁷Al dipolar interactions in solids, comparison with TRAPDOR, van Wüllen and Kalwei, 139, 250

deuterium, principles and applications for distance measurements, Sack *et al.*, **138**, 54

distances from heterospins to clusters of ¹³C labels determined by, Schaefer, 137, 272

and θ-REDOR, comparison for measuring ¹³C-²D dipolar interactions in solids, Gullion, **139**, 402

 θ -REDOR

and REDOR, comparison for measuring ¹³C-²D dipolar interactions in solids, Gullion, **139**, 402

Reentrant resonator

tunable, with transverse orientation of electric field, for *in vivo* EPR spectroscopy, Chzhan *et al.*, **137**, 373

Reference deconvolution

in frequency domain, Goez and Heun, 136, 69

Refocusing

efficient, one-spin and two-spin interactions for NMR quantum computation, Jones and Knill, 141, 322

Relaxation (see also Cross-relaxation; Spin-lattice relaxation; Spin-spin relaxation)

CSA/DD cross-correlated, comparison of 1D and 2D (unbiased) experimental methods for measuring, Batta, Kövér, and Kowalewski, 136, 37

data, estimation of dynamic parameters from, using Lipari–Szabo modelfree approach and Bayesian statistical methods, Andrec, Montelione, and Levy, **139**, 408

effects, in system of spin- $\frac{1}{2}$ nucleus coupled to quadrupolar spin subjected to RF irradiation, Smith and Murali, 136, 27

heteronuclear, bias estimation: method for determining B_1 field inhomogeneity, Guenneugues, Berthault, and Desvaux, 136, 118

in multipolar AX systems under spin locking conditions, Kaikkonen and Kowalewski, **141**, 326

Relaxation NMRI

selective imaging of biofilms in porous media by, Hoskins et al., 139, 67 Relaxation rate

multinuclear, of clay suspensions, Grandjean and Robert, 138, 43

 $N^{\rm H}$ and H^{α} backbone protons in proteins, measurement, Millet *et al.*, 139, 434

Relaxation time

rotating frame and longitudinal, measurement through fully *J*-decoupled homonuclear spectra, Guenneau *et al.*, **140**, 250

and state of water in gelatin gels, Vackier, Hills, and Rutledge, **138**, 36 in unresolved NMR spectra, SPORT-NMR software for, Geppi and Forte, **137**, 177

Residual dipolar coupling

 13 C $^{\alpha}$ - 1 H $^{\alpha}$, in 15 N/ 13 C-labeled proteins, J^{CH} -modulated 2D (HACACO)NH pulse scheme for quantitative measurement, Hitchens, McCallum, and Rule, **140**, 281

in crosslinked elastomers, ¹H NMR imaging, Schneider, Demco, and Blümich, **140**, 432

H^N-H^α, measurement in proteins, Cai *et al.*, **139**, 451

order matrix analysis using singular value decomposition, Losonczi *et al.*, **138**, 334

Resin

peptide bound to, under MAS, origin of residual NMR linewidth of, Elbayed et al., 136, 127

Resolution

in high-field echo planar microscopy, Peters and Bowtell, 137, 196 Resolution enhancement

in ¹³C and ¹⁵N magic-angle turning experiments with TPPM decoupling, McGeorge, Alderman, and Grant, **137**, 138

Resonance assignment (see also Assignment)

determination of multiple ϕ -torsion angles in proteins by selective and extensive ¹³C labeling and 2D solid-state NMR, Hong, **139**, 389

photoactive yellow protein photointermediates, NMR experiments for, Rubinstenn *et al.*, **137**, 443

sensitivity-enhanced sim-CT HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH triple-resonance experiments, Swapna and Montelione, 137, 437

triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in ¹³C, ¹⁵N-labeled RNA, Wöhnert *et al.*, **139**, 430

Resonance structure

multiple-frequency, high-field DNP and ENDOR with, Weis et al., 140, 293 Resonant frequency

300 to 900 MHz, in constant microwave field, EDMR signal intensity at, Sato et al., 139, 422

Resonator

for high-field DNP and ENDOR: novel multiple-frequency resonance structure, Weis et al., 140, 293

RF, and openable high-strength gradient set, for orthopedic MRI, Crozier *et al.*, **139**, 81

tunable reentrant, with transverse orientation of electric field, for *in vivo* EPR spectroscopy, Chzhan *et al.*, **137**, 373

Restricted diffusion

under generalized gradient waveforms, spin echo analysis: porous media, Codd and Callaghan, 137, 358

MRI edge enhancement as diffusive discord of spin phase structure, Stepišnik et al., 137, 154

permeability coefficients from NMR *q*-space data: models with unevenly spaced semipermeable parallel membranes, Kuchel and Durrant, **139**, 258

theory of spin echo in restricted geometries under stepwise gradient pulse sequence, Barzykin, 139, 342

Retinal

¹³C-labeled, anomalous rotational resonance spectra in MAS NMR, Helmle et al., 140, 379

RFDR

¹³C distance measurements in p-xylene/Dianin's inclusion compound by, Zaborowski, Zimmermann, and Vega, 136, 47

Ribonucleotide reductase

E. coli, tyrosyl radical of, pulsed ENDOR at 140 GHz, Bennati et al., 138, 232

RNA

¹³C, ¹⁵N-labeled, triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in, Wöhnert *et al.*, **139**, 430

ROESY

off-resonance, tilt angle dependence of cross-relaxation in, Cutting, Ghose, and Bodenhausen, 138, 326

3D ¹⁵N-edited HMQC and HSQC, signal enhancement using 45° water flipback, Gruschus and Ferretti, **140**, 451

Rotating frame

proton spin magnetization in, spectroscopy from: study of small tunneling splitting, Damyanovich, Peternelj, and Pintar, **140**, 9

Rotating-frame NQR

phase-modulated, for spatial encoding, Casanova, Robert, and Pusiol, 141,

Rotating-frame Overhauser effect spectroscopy (see ROESY)

Rotating solids

efficient spectral simulations in NMR: γ-COMPUTE, Hohwy *et al.*, **136**, 6 Rotational echo double resonance (*see* REDOR)

Rotational resonance

anomalous spectra, in MAS NMR, Helmle et al., 140, 379

constant-time, for solid-state NMR distance measurements on large biomolecules, Balazs and Thompson, 139, 371

MAS NMR lineshapes of four-¹³C-spin system, magnitudes and orientations of interaction tensors determined from, Dusold, Maisel, and Sebald, **141**, 78

S

Saponite

and laponite, suspensions, ⁷Li double-quantum filtered NMR and multinuclear relaxation rates, Grandjean and Robert, **138**, 43

SBM theory

paramagnetic relaxation enhancement of low-symmetry complexes for electron spin quantum number $S=\frac{5}{2}$, Strandberg and Westlund, **137**, 333 Scalar interactions

and dipolar interactions, role in paramagnetic effects on nuclear relaxation in enzyme-bound Co(II)-adenine nucleotide complexes, Ray, Jarori, and Nageswara Rao, 136, 130

Scalar measures

used in MR diffusion tensor imaging, comparison, Bahn, 139, 1

S³CT (see Spin-state-selective coherence transfer)

S³E (see Spin-state-selective excitation)

SEFT

and APT, modifications, and ORSAT: ¹³C signal assignment, Beckmann, Dietrich, and Radeglia, **137**, 132

Selective excitation

offset profiles of selective pulses in isotopically labeled macromolecules, Eykyn, Ghose, and Bodenhausen, 136, 211

proton signals in NMR of isotopically labeled macromolecules, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

Selective heteronuclear cross polarization

selective excitation of proton signals in NMR of isotopically labeled macromolecules, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

Selective heteronuclear J cross polarization

mixing sequences for: PRAWN, Chandrakumar and Kimmich, ${\bf 137,}\ 100$ Selective NOE

identification of spin diffusion pathways in isotopically labeled biomolecules, Eykyn, Früh, and Bodenhausen, **138**, 330

Selective polarization

¹³C, in lipid bilayer-bound polypeptide by solid-state NMR, Tian, Fu, and Cross, 139, 377

Selective pulses

band-selective HSQC and HMBC experiments using excitation sculpting and PFGSE, Gaillet et al., 139, 454

in isotopically labeled macromolecules, offset profiles of, Eykyn, Ghose, and Bodenhausen, ${\bf 136},\,{\bf 211}$

Selective spin inversion

asymmetric adiabatic pulses for NH selection, Hwang, van Zijl, and Garwood, 138, 173

Self-correcting distance geometry

based NOAH/DIAMOD programs, automated 2D NOESY assignment and structure calculation of crambin with, Xu et al., 136, 76

Self-diffusion coefficients

maps, by RF field gradient NMR microscopy, Valtier, Humbert, and Canet, 141, 7

Self-diffusion imaging

by spin echo in Earth's magnetic field, Mohorič *et al.*, **136**, 22 Sensitivity

and sign discrimination and isotropic mixing, in solid-state wideline heteronuclear correlation experiments, Oliver and Titman, 140, 235

Sensitivity-enhanced HSQC

artifacts in, Turner, Connolly, and Stern, 137, 281

Sensitivity enhancement

observation of long-range small-molecule NOEs using, Van, Smith, and Shaka, **141**, 191

transverse relaxation-optimized spectroscopy, Rance, Loria, and Palmer, 136, 92

Sequential rephasing

by pulsed-field gradients, time correlations in fluid transport obtained by, Stapf, Damion, and Packer, 137, 316

Shell eggs

application of low-frequency ¹H NMR external unit for analysis of large foodstuff samples, Capozzi *et al.*, **138**, 277

Short echo time

¹H NMR spectra of rat brain, in vivo quantification of 18 metabolites, Pfeuffer et al., 141, 104

²⁹Si

triphenylsilane, CSA/DD cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

Sidebands

residual, elimination in BEST homonuclear adiabatic decoupling for ¹³C- and ¹⁵N-double-labeled proteins, Zhang and Gorenstein, **138**, 281

and ¹³⁹La NMR application: multiple-rotor-cycle QPASS pulse sequences, Aurentz *et al.*, **138**, 320

Side chair

sites, of amino acids and peptides, application of 2D and 3D $^{1}H/^{13}C$ PISEMA experiments, Gu and Opella, **140**, 340

Side-chain dynamics

Sideband separation

nitroxide, in spin-labeled helix-forming peptide, by high-frequency EPR, Bennati et al., 139, 281

Sign

heteronuclear coupling constants in transition metal complexes, measurement, Otting, Soler, and Messerle, 137, 413; erratum, 139, 186

Signal enhancement

using 45° water flipback, for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

Signal increase

functional MR imaging of human brain using FLASH, effects of imaging parameters, Preibisch and Haase, **140**, 162

Signal intensity

in FLASH-EPI-Hybrid sequences, Hillenbrand et al., 139, 74

Signal leakage

unwanted, in excitation sculpting with single axis gradients, Jerschow, 137, 206

Signal-to-noise ratio

absolute EPR spin-echo and noise intensities, Rinard et al., 140, 69

EPR, frequency dependence, Rinard et al., 140, 218

in FLASH-EPI-Hybrid sequences: signal intensities, Hillenbrand *et al.*, **139**, 74

Signal selection

in high-resolution NMR by pulsed-field gradients design of gradient pulse sequences, Thomas *et al.*, **137**, 10 geometrical analysis, Mitschang, **137**, 1

Sign discrimination

and sensitivity and isotropic mixing, in solid-state wideline heteronuclear correlation experiments, Oliver and Titman, 140, 235

Simulated annealing

fast optimization of biplanar gradient coil set, Tomasi et al., 140, 325 Simulation

EPR spectra of spin labels in liquids

experimental, Robinson, Mailer, and Reese, 138, 210

theory and data analysis, Robinson, Mailer, and Reese, 138, 199

exact product operator evolution of weakly coupled spin- $\frac{1}{2}$ I_mS_n systems during arbitrary RF irradiation of I spins, Skinner and Bendall, **141**, 271 magnetic resonance static powder lineshapes, Ponti, **138**, 288

numerical

analysis of *J* coupling-induced fat suppression in DIET imaging, Stables *et al.*, **136**, 143

density matrix, of effects of J coupling in spin-echo and fast spin-echo imaging, Stables *et al.*, **140**, 305

one- and two-dimensional spectra, pulsed-field gradients in, Meresi *et al.*, **137.** 186

polycrystalline EPR spectrum, Misra, 137, 83

Simultaneous constant-time period

sensitivity-enhanced HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH triple-resonance experiments, Swapna and Montelione, 137, 437

Single-point ramped imaging with T_1 enhancement (SPRITE) MRI gases, Prado *et al.*, **137**, 324

with prepared magnetization and centric *k*-space sampling, Mastikhin *et al.*, **136.** 159

Single-shot diffusion measurement

in laser-polarized gas, Peled et al., 140, 320

Single-shot experiments

for acquisition of coherence-transfer functions in real time, Luy and Glaser, 138, 187

Single-shot imaging

LSI, using stimulated echoes, Finsterbusch and Frahm, 137, 144 Single-turn coil

electrically detected magnetic resonance signal intensities at resonant frequencies from 300 to 900 MHz in constant microwave field, Sato *et al.*, **139**, 422

Singular-value decomposition

order matrix analysis of residual dipolar couplings using, Losonczi *et al.*, **138**, 334

Sinusoidal gradient

magic echo solid-state NMR imaging without rapidly switchable field gradient, Matsui et al., 138, 220

Site exchange

slow site exchange processes in solution NMR: continuous Gaussian exchange model, Schurr *et al.*, **140**, 404

Skeletal muscle

creatine resonances in ¹H MR spectra of, effect of exercise (human), Kreis et al., 137, 350

lactate in, anisotropic orientation observed by dipolar coupling in ¹H NMR, Asllani *et al.*, **139**, 213

Skewness

invariant and orthonormal scalar measures derived from MR diffusion tensor imaging, Bahn, **141**, 68

Slaved pulses

evaluation for study of protein hydration, Bornet, Guerlesquin, and Piotto, 138, 107

SLOOP

beyond k-space: spectral localization using higher-order gradients, Pohmann, Rommel, and von Kienlin, 141, 197

Slow chemical exchange

in NMR, selective injection of magnetization by, Boulat, Epstein, and Rance, 138, 268

119St

chemical shift thermometer Sm₂Sn₂O₇, in temperature calibration under ultrafast MAS conditions, Langer *et al.*, **138**, 182

Sodium

ions, in ordered environments in biological systems, analysis of ²³Na NMR spectra, Kemp-Harper, Wickstead, and Wimperis, **140**, 351

triple-quantum-filtered twisted projection sodium MRI of human articular cartilage *in vivo*, Borthakur *et al.*, **141**, 286

Sodium chloride

changes in ionic concentrations during dissolving of, monitoring with MR current density imaging, Beravs, Demšar, and Demsar, 137, 253

Software

spreadsheet, lineshape calculations on, Mayer, 138, 1 Solids

¹³C-²⁷Al dipolar interactions in, ¹³C-²⁷Al TRAPDOR and REDOR experiments for detection of, van Wüllen and Kalwei, **139**, 250

magnetically dilute, $S = \frac{1}{2}$ molecular species in, electron spin lattice relaxation rates at temperatures 10–300 K, Zhou *et al.*, **139**, 165

polymers, $T_{2\rho}$ -contrasted NMR images, De Luca et al., 139, 126

rotating, efficient spectral simulations in NMR: γ -COMPUTE, Hohwy *et al.*, **136**, 6

Solid-state NMR

accuracy of distance measurements in, Hodgkinson and Emsley, **139**, 46 ¹³C selective polarization and spin diffusion in lipid bilayer-bound polypeptide by, Tian, Fu, and Cross, **139**, 377

dipolar INADEQUATE, with large double-quantum spectral width, Hong, 136, 86

distance measurements on large biomolecules, practical methods: constanttime rotational resonance, Balazs and Thompson, 139, 371

¹⁹F magic-angle-turning experiments with multiple-pulse homonuclear decoupling, Hughes, Brouwer, and Harris, 138, 256

homonuclear two spin-½ system, analysis of dipolar coupling-mediated coherence transfer in, Taylor and Ramamoorthy, **141**, 18

INADEQUATE-CR experiments, Verel, van Beek, and Meier, **140**, 300 membrane-associated peptides, lanthanide chelates as bilayer alignment tools in, Prosser *et al.*, **141**, 256

multipulse, on static and oriented systems, structural parameters from ¹⁹F homonuclear dipolar couplings by, Grage and Ulrich, **138**, 98

narrowband excitation of ²H powder pattern and application to ²H 1D exchange sample-turning NMR, Reichert et al.n, 139, 308

off-resonance multiple-pulse dynamics: revised coherent averaging theory analysis, Cho, 141, 164

3PbO-2P₂O₅ glass, in analysis of chemical bonding of lead via isotropic vs anisotropic correlation: PASS shifted echo, Fayon *et al.*, **137**, 116

quadrupolar and chemical shift tensors characterized by 2D multiple-quantum NMR spectroscopy, Medek and Frydman, 138, 298

selection rules for multiple-quantum NMR excitation, Tycko, **139**, 302 three-dimensional ¹³C shift/¹H–¹⁵N coupling/¹⁵N shift NMR correlation spectroscopy, Gu and Opella, **138**, 193

two-dimensional

[1-15N]-2'-deoxyguanosine, magnitudes and orientations of ¹⁵N chemical shift determined on polycrystalline sample by, Lorigan *et al.*, **140**, 315 and selective and extensive ¹³C labeling, in determination of multiple φ-torsion angles in proteins, Hong, **139**, 389

two- and three-dimensional 1 H/ 13 C PISEMA experiments and application to backbone and side chain sites of amino acids and peptides, Gu and Opella, **140**, 340

Solid-state NMR correlation spectroscopy

multidimensional, experimental aspects, Ramamoorthy, Wu, and Opella, 140, 131

Solid-state NMR imaging

magic echo, without rapidly switchable field gradient, Matsui *et al.*, **138**, 220 Solution NMR

slow site exchange processes: continuous Gaussian exchange model, Schurr et al., 140, 404

Solution structure

determination: observation of long-range small-molecule NOEs using sensitivity enhancement scheme, Van, Smith, and Shaka, **141**, 191

Solvent dependence

spin-echo dephasing for chromium(V) and vanadyl complexes in glassy solution, Eaton and Eaton, 136, 63

Solvent suppression

finite impulse response filter design for accurate quantification of ¹H spectra, Sundin *et al.*, **139**, 189

SORC sequence

feedback optimization of offset frequency, Blauch, Schiano, and Ginsberg, 139, 139

feedback optimization of pulse width, Schiano et al., 140, 84

Spatial encoding

phase-modulated rotating frame NQR techniques for, Casanova, Robert, and Pusiol, **141**, 62

Spatially localized NMR spectroscopy

stimulated anti-echo selection in, Zhu and Smith, 136, 1

Spatial resolution spectroscopy

simultaneous micromechanical and electromagnetic detection in EPR, Alzetta et al., 141, 148

Spectral analysis

bilinear Bayesian spectral decomposition, Ochs et al., 137, 161 Spectral fitting

NMR spectra, using alternating optimization method with *a priori* knowledge, Bi *et al.*, **140**, 108

Spectral localization with optimal pointspread function

beyond k-space: spectral localization using higher-order gradients, Pohmann, Rommel, and von Kienlin, 141, 197

Spectral simulation

efficient, in NMR of rotating solids: γ -COMPUTE, Hohwy *et al.*, **136**, 6 incorporating gradient coherence selection, Young *et al.*, **140**, 146 magnetic resonance static powder lineshapes, Ponti, **138**, 288

Spectrometer

transient MR without RF field pulses: fast field switching, Sloop, Lin, and Ackerman, 139, 60

Spherical code

quantitative assessment: simulation of MR static powder lineshapes, Ponti, 138, 288

Spin coherence relaxation

in rotating frame, as microscopy parameter for strongly coupled spin systems, De Luca et al., 139, 126

Spin concentration

in possible ESR dosimeter: electron spin echo study of X-irradiated ammonium tartrate, Brustolon, Zoleo, and Lund, 137, 389

Spin counting

with fast MAS, Geen et al., 138, 167

Spin diffusion

attenuation of cross-peak intensities in QUIET–BIRD–NOESY, Cutting and Bodenhausen, **140**, 289

¹³C, in lipid bilayer-bound polypeptide, by solid-state NMR, Tian, Fu, and Cross, 139, 377

effects, measuring long-range nuclear Overhauser enhancements free of, Harris $\it{et~al.},\, 140,\, 504$

¹H, and reduced ¹³C exchange, combined 4D experiment for determining length scale of dynamic heterogeneities, Tracht *et al.*, **140**, 460

high-order mechanisms, in $^{19}\mathrm{F}$ 2D NMR of oxyfluorides, Du, Levitt, and Grey, $140,\,242$

in liquid-state NMR, experimental control: comparison of methods, Boulat, 139, 354

pathways, identification in isotopically labeled biomolecules, Eykyn, Früh, and Bodenhausen, 138, 330

and quantitative measurement of longitudinal and transverse cross-relaxation rates, Malliavin *et al.*, **140**, 189

⁸⁷Rb, in ferroelectric RbH₂PO₄ studied by 2D exchange NMR, Cereghetti and Kind, 138, 12

removing effects of, in solid-state wideline heteronuclear correlation experiments, Oliver and Titman, 140, 235

Spin echo

conditions for exponential time-cubed echo delays, Pfitsch, McDowell, and Conradi, 139, 364

in Earth's magnetic field, self-diffusion imaging by, Mohorič *et al.*, **136**, 22 efficient refocusing of one-spin and two-spin interactions for NMR quantum computation, Jones and Knill, **141**, 322

MRI edge enhancement as diffusive discord of spin phase structure, Stepišnik *et al.*, **137**, 154 theory of, in restricted geometries under stepwise gradient pulse sequence, Barzykin, **139**, 342

Spin-echo analysis

restricted diffusion under generalized gradient waveforms: porous media, Codd and Callaghan, 137, 358

Spin-echo decay

and slow site exchange processes in solution NMR, Schurr et al., 140, 404 Spin-echo dephasing

for chromium(V) and vanadyl complexes in glassy solution, solvent and temperature dependence, Eaton and Eaton, 136, 63

Spin-echo imaging

effects of *J* coupling, density matrix simulations, Stables *et al.*, **140**, 305 Spin exchange

²H 1D exchange sample-turning NMR, application of narrowband excitation of ²H powder pattern, Reichert *et al.*, **139**, 308

at the magic angle, multidimensional solid-state NMR experiments incorporating, experimental aspects, Ramamoorthy, Wu, and Opella, **140**, 131

Spin Hamiltonian

numerical diagonalization of, modeling EPR powder spectra using, Morin and Bonnin, 136, 176

parameters, from polycrystalline EPR spectrum, evaluation, Misra, **140**, 179 Spin labels

in liquids, linewidth analysis

experimental, Robinson, Mailer, and Reese, 138, 210

theory and data analysis, Robinson, Mailer, and Reese, 138, 199

nitroxide, helix-forming peptide labeled with, nitroxide side-chain dynamics by high-frequency EPR, Bennati *et al.*, **139**, 281

Spin-lattice relaxation

in enzyme-bound Co(II)-adenine nucleotide complexes, paramagnetic effects: role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

images, by RF field gradients, Humbert et al., 138, 164

⁷Li, evidence for competition between Na⁺ and Li⁺ for unsealed and cytoskeleton-depleted RBC membrane, Srinivasan et al., 140, 206

measurement through fully *J*-decoupled homonuclear spectra, Guenneau $\it et$ $\it al., 140, 250$

selective imaging of biofilms in porous media, Hoskins *et al.*, **139**, 67 ¹²⁹Xe in blood, and role of oxygenation, Albert *et al.*, **140**, 264 Spin locking

NMR relaxation in multipolar AX systems under, Kaikkonen and Kowalewski, **141**, 326

Spin magnetization

proton, in rotating frame, spectroscopy from: study of small tunneling splitting, Damyanovich, Peternelj, and Pintar, **140**, 9

Spinning-sideband patterns

in recoupled polarization transfer heteronuclear ¹H–¹³C multiple-quantum correlation in solids under ultra-fast MAS, Saalwächter, Graf, and Spiess, **140**, 471

Spin phase structure

MRI edge enhancement as diffusive discord of, Stepišnik et al., 137, 154 Spin probes

high-resolution magnetic relaxation dispersion measurements using dualmagnet system, Wagner et al., 140, 172

Spin relaxation

in enzyme-bound Co(II)-adenine nucleotide complexes, paramagnetic effects: role of dipolar and scalar interactions, Ray, Jarori, and Nageswara Rao, 136, 130

Spins

four coupled spins $\frac{1}{2}$ under isotropic mixing conditions, analytical polarization transfer functions for, Luy, Schedletzky, and Glaser, 138, 19

 $I = \frac{1}{2}$

coupled to quadruolar nuclei in liquids, line narrowing: effects of weak decoupling fields, Bendel and Baram, 141, 121

nuclear quadrupole resonance, calculations of multipulse sequence in, Odin, **141**, 239

Spin-spin coupling (see J-coupling)

Spin-spin relaxation

conditions for exponential time-cubed echo delays, Pfitsch, McDowell, and Conradi, 139, 364

in rotating frame, as microscopy parameter for strongly coupled spin systems, De Luca *et al.*, **139**, 126

selective imaging of biofilms in porous media, Hoskins *et al.*, **139**, 67 susceptibility-induced shortening, corrected equations for, Gillis, Roch, and Brooks, **137**, 402

Spin-state-selective coherence transfer

 13 C natural abundance experiments for measurement of *J*-coupling constants between 13 C $^{\alpha}$ or 1 H $^{\alpha}$ and other protons in protein, Sørensen, Meissner, and Sørensen, **137**, 237

efficiency, role in design of TROSY-type multidimensional NMR experiments, Meissner and Sørensen, 139, 439

pulse sequences for measurement of one-bond ¹⁵N-¹H coupling constants in protein backbone, Lerche *et al.*, **140**, 259

suppression of diagonal peaks in TROSY-type ¹H NMR NOESY spectra of ¹⁵N-labeled proteins, Meissner and Sørensen, **140**, 499

Spin-state-selective excitation

 13 C natural abundance experiments for measurement of *J*-coupling constants between 13 C $^{\alpha}$ or 1 H $^{\alpha}$ and other protons in protein, Sørensen, Meissner, and Sørensen, 137, 237

suppression of diagonal peaks in TROSY-type ¹H NMR NOESY spectra of ¹⁵N-labeled proteins, Meissner and Sørensen, **140**, 499

Spin-state-selective filters

double-/zero-quantum 2D NMR spectra simplified by, in measurement of homonuclear ²*J*-couplings, Permi *et al.*, **139**, 273

measurement of $^1J_{\rm NC'}$ and $^2J_{\rm H^NC'}$ couplings from 2D correlation spectrum, Permi $\it et~al.,~140,~32$

Spin-state-selective time-proportional phase incrementation (S³ TPPI)

optimization of 3D HCCH TROSY-type NMR correlation of aromatic $^{1}\text{H}^{-13}\text{C}$ groups in proteins, Meissner and Sørensen, **139**, 447 suppression of heteronuclear coupling constants in multidimensional NMR,

Schulte-Herbrüggen et al., 139, 443

Spin systems

four-¹³C-spin system, interaction tensors determined from rotational resonance MAS NMR lineshapes of, magnitudes and orientations, Dusold, Maisel, and Sebald. **141**, 78

general AMX, under isotropic mixing, analytical coherence-transfer functions for, Schedletzky and Glaser, 123A, 174; erratum, 136, 134

homonuclear two spin-½ solid-state, analysis of dipolar coupling-mediated coherence transfer in, Taylor and Ramamoorthy, **141**, 18

multipolar AX, under spin locking conditions, NMR relaxation in, Kaikkonen and Kowalewski, **141**, 326

spin-½ nucleus coupled to quadrupolar spin subjected to RF irradiation, relaxation effects in, Smith and Murali, 136, 27

spin-\(\frac{5}{2}\), high-resolution heteronuclear correlation spectrum, Chan, **140**, 487 two-spin, construction and implementation of NMR quantum logic gates for, Price *et al.*, **140**, 371

weakly coupled spin- $\frac{1}{2}$ I_mS_n systems, exact product operator evolution during arbitrary RF irradiation

of I spins, Skinner and Bendall, 141, 271

of one spin: J pulses for multiplet-selective NMR, Bendall and Skinner, **141**, 261

Spin thermodynamics

based analysis of cross-polarization dynamics between ¹⁹F and ¹H, Ando, Harris, and Reinsberg, **141**, 91

Spiral MR

gradient design, simple reliable solutions for, Salustri, Yang, and Glover, 140, 347

Splitting

small tunneling splitting: spectroscopy from proton spin magnetization in rotating frame, Damyanovich, Peterneli, and Pintar, **140**, 9

SPORT-NMR software

for determination of relaxation times in unresolved NMR spectra, Geppi and Forte. 137, 177

Spreadsheet software

lineshape calculations on, Mayer, 138, 1

SPRITE (single-point ramped imaging with T_1 enhancement) MRI gases, Prado *et al.*, **137**, 324

with prepared magnetization and centric k-space sampling, Mastikhin et al., 136, 159

Static powder lineshape

simulation, Ponti, 138, 288

STEAM

spectral simulations incorporating gradient coherence selection, Young et al., 140, 146

Stimulated anti-echo

selection, in spatially localized NMR spectroscopy, Zhu and Smith, 136, 1 Stimulated echo

displacement encoding with, in cardiac functional MRI: DENSE, Aletras *et al.*, **137**, 247

fast-DENSE high-resolution strain analysis of human heart, Aletras, Balaban, and Wen, **140**, 41

SE-enhanced double-quantum filter, simultaneous lactate editing and observation of other metabolites using, Lei and Peeling, 137, 215

single-shot line scan imaging using, Finsterbusch and Frahm, **137**, 144 Stimulated echo acquisition mode (STEAM)

stimulated anti-echo selection in spatially localized NMR spectroscopy, Zhu and Smith, 136, 1

Stone's perturbation theory

and configuration interaction, g-matrix based on, Li et al., 138, 74

Stopped-flow EPR

rapid scan, dielectric resonator-based, Sienkiewicz et al., 136, 137

 $\mbox{S}^{\mbox{\scriptsize 3}}$ TPPI (see Spin-state-selective time-proportional phase incrementation) Strain analysis

high-resolution, of human heart, with fast-DENSE, Aletras, Balaban, and Wen, 140, 41

Stray field imaging

high-gradient permanent magnet for profiling of planar films and coatings, Glover et al., 139, 90

Stroke

murine focal cerebral ischemia models, application of high-resolution MR angiography of mouse brain, Beckmann, Stirnimann, and Bochelen, **140**, 442

Strong coupling

ABX strong coupling signals, suppression in heteronuclear scalar and dipolar correlation spectra, Kövér and Batta, 138, 89

spin systems with, spin coherence relaxation in rotating frame as microscopy parameter for, De Luca *et al.*, **139**, 126

Strong off-resonant comb sequence

feedback optimization of offset frequency, Blauch, Schiano, and Ginsberg, 139, 139

feedback optimization of pulse width, Schiano et al., 140, 84

Structural relationships

macromolecular ligands, mapping approach: theoretical analysis of interligand Overhauser effect, London, 141, 301

Structure

crambin, calculation with self-correcting distance gemometry-based NOAH/ DIAMOD programs, Xu et al., 136, 76

2D { 31 P} spin-echo-difference constant-time [13 C, 1 H] HMQC experiment for simultaneous determination of $^{3}J_{\text{H3'P}}$ and $^{3}J_{\text{C4'P}}$ in 13 C-labeled nucleic acids and protein complexes, Szyperski *et al.*, **140**, 491

dual processing of 2D exchange data in MAS NMR of solids, Tycko and Berger, 141, 141

mixed proteins in biological buffer solutions, capillary array electrophoretic NMR study, He *et al.*, **141**, 355

Sulfur hexafluoride

¹⁹F, gas MRI: single-point ramped imaging with T₁ enhancement (SPRITE), Prado et al., 137, 324

Superparamagnetic particles

susceptibility-induced T_2 shortening due to, corrected equations for, Gillis, Roch, and Brooks, 137, 402

Suppression

diagonal peak, in TROSY-type ¹H NMR NOESY spectra of ¹⁵N-labeled proteins, Meissner and Sørensen, **140**, 499

fat, J coupling-induced, in DIET imaging, Stables et al., 136, 143

macromolecule resonances in short-echo-time ¹H NMR spectroscopy of human brain, application of multiple inversion recovery, Knight-Scott, **140**, 228

radiation damping: signal enhancement using 45° water flipback for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

solvent: finite impulse response filter design for accurate quantification of ¹H spectra, Sundin *et al.*, **139**, 189

systematic F₁ artifacts in 2D NMR, randomized acquisition for, Bowyer, Swanson, and Morris, **140**, 513

Surface charge

method for computing induced magnetic field in trabecular bone, evaluation, Hwang and Wehrli, 139, 35

Surface-sensitive imaging

Xenon-131, of aerogels in liquid xenon near critical point, Pavlovskaya et al., 137, 258

Susceptibility-induced relaxation

T₂, corrected equations for, Gillis, Roch, and Brooks, 137, 402

Synchronous nutation

selective injection of magnetization by slow chemical exchange in NMR, Boulat, Epstein, and Rance, 138, 268

Т

 T_1 (see Spin-lattice relaxation)

 T_2 (see Spin-spin relaxation)

 T_2^*

 T_2^* -weighted image contrast, magnetic susceptibility artifacts in, microimaging at 14 T using GESEPI for removal of, Yang *et al.*, **141**, 1

TAM radical

water doped with, ¹H DNP at 1.4 T, Wind and Ardenkjær-Larsen, **141**, 347 Target field method

design of magic angle gradient coils, Barbara and Bronnimann, 140, 285 Temperature calibration

under ultrafast MAS conditions, Langer et al., 138, 182

Temperature dependence

electron spin lattice relaxation rates for $S = \frac{1}{2}$ molecular species in glassy matrices or magnetically dilute solids between 10 and 300 K, Zhou *et al.*, **139**, 165

spin-echo dephasing for chromium(V) and vanadyl complexes in glassy solution, Eaton and Eaton, 136, 63

Temperature imaging

and convection measurement, in liquid samples, Loening and Keeler, 139, 334

Temperature variation

systematic F_1 artifacts in 2D NMR from, randomized acquisition for suppression of, Bowyer, Swanson, and Morris, **140**, 513

Tendor

²³Na NMR spectra (pig), Kemp-Harper, Wickstead, and Wimperis, **140**, 351 water molecules in, dipolar interactions and dynamic processes, ¹H and ²H

homonuclear and heteronuclear MQF NMR study (bovine), Eliav and Navon. 137, 295

Tensor operators

generation of operator equivalents and calculation of matrix elements, Ryabov, **140**, 141

p-Terphenyl

crystals, triplet state of pentacene in, dynamic nuclear polarization in pulsed ENDOR, Kouskov *et al.*, **137**, 25

Three-dimensional NMR

¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, 138, 193

¹H/¹³C PISEMA experiments and application to backbone and side chain sites of amino acids and peptides, Gu and Opella, **140**, 340

¹⁵N-edited ROESY and NOESY HMQC and HSQC, signal enhancement using 45° water flipback for, Gruschus and Ferretti, 140, 451

3D-NOESY-HSQC

¹³C or ¹⁵N edited spectra, using back-calculated and experimental spectra, computer-assisted assignment by, Görler et al., 137, 39

Through-bond correlation

thymine resonances in ¹³C-labeled DNA oligonucleotides, HCCCH experiment for, Sklenář, Masse, and Feigon, **137**, 345

Thymine

resonances in ¹³C-labeled DNA oligonucleotides, HCCCH experiment for through-bond correlation of, Sklenář, Masse, and Feigon, **137**, 345

Ti3+ center

large-magnitude high-spin nuclear parameters in, from X-band EPR measurements at 10 K, Tennant and Claridge, 137, 122

Tilt angle

dependence of cross-relaxation in off-resonance ROESY on, Cutting, Ghose, and Bodenhausen, 138, 326

Tilting

active-coupling-pattern, pure-phase homonuclear *J*-modulated HMQC with, for determination of homonuclear coupling constants, Koźmiński, **141**, 185

Time correlations

in fluid transport, obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

Time-cubed echo delays

exponential, conditions for, Pfitsch, McDowell, and Conradi, 139, 364 Time domain

time-domain quantification of series of biomedical MR spectroscopy signals, Vanhamme et al., 140, 120

Time-domain EPR spectroscopy/imaging

RF, high-speed data acquisition system and receiver configurations, Subramanian *et al.*, **137**, 379

Time-domain NMR

relaxation study of state of water in gelatin gels, Vackier, Hills, and Rutledge, 138, 36

spectral fitting using alternating optimization method with *a priori* knowledge, Bi *et al.*, **140**, 108

Time-reversal symmetry

derivation of selection rules for multiple-quantum NMR excitation in solids from, Tycko, **139**, 302

 t_1 noise

incoherent, conversion of coherent artifacts into: randomized acquisition for suppression of artifacts in 2D NMR, Bowyer, Swanson, and Morris, 140, 513

TOCSY

analytical polarization transfer functions for four coupled spins ½ under isotropic mixing conditions, Luy, Schedletzky, and Glaser, **138**, 19

HCCCH experiment for through-bond correlation of thymine resonances in ¹³C-labeled DNA oligonucleotides, Sklenář, Masse, and Feigon, **137**, 345

PFG- ω_1 -filtered, Xu, Zhang, and Evans, **138**, 127

selective excitation of proton signals in isotopically labeled macromolecules, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

simplified multiplet pattern HSQC-TOCSY for determination of long-range heteronuclear coupling constants, Koźmiński, 137, 408

single-shot experiments for acquisition of coherence-transfer functions in real time, Luy and Glaser, 138, 187

Torsion angles

³*J*(H3'_i, P_{i+1}) and ³*J*(H5'_i/5"_i, P_i) coupling constants in ¹³C-labeled nucleic acids, determination using CT-HMQC, Hu *et al.*, **139**, 181

multiple ϕ -torsion angles in proteins, determination by selective and extensive ¹³C labeling and 2D solid-state NMR, Hong, **139**, 389

TOSS

magic-angle spinning NMR spectroscopy with composite pulses, Leppert, Heise, and Ramachandran, 139, 382

Total correlation spectroscopy (see TOCSY)

TPPM decoupling

¹³C and ¹⁵N magic-angle turning with, resolution enhancement in, Mc-George, Alderman, and Grant, 137, 138

Transfer of populations in double resonance (see TRAPDOR)

Transition metal centers

application of W-band pulsed ENDOR spectrometer, Gromov et al., 139, 8 Transition metal complexes

magnitude and sign of heteronuclear coupling constants in, measurement, Otting, Soler, and Messerle, 137, 413; *erratum*, 139, 186

S = $\frac{1}{2}$, in glassy matrices or magnetically dilute solids, electron spin lattice relaxation rates at temperatures 10–300 K, Zhou *et al.*, **139**, 165

Transverse cross relaxation

¹H, in ¹H-¹⁵N correlated ¹H CPMG experiments, Ishima, Louis, and Torchia, 137, 289

Transversely oriented electric field

tunable reentrant resonator with, for *in vivo* EPR spectroscopy, Chzhan *et al.*, **137**, 373

Transverse relaxation (see Spin-spin relaxation)

Transverse relaxation-optimized spectroscopy (see TROSY)

TRAPDOR

¹³C-²⁷Al, for detection of ¹³C-²⁷Al dipolar interactions in solids, comparison with REDOR, van Wüllen and Kalwei, 139, 250

Trehalose

CSA/DD cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

Triarylmethyl radical

water doped with, ¹H DNP at 1.4 T, Wind and Ardenkjær-Larsen, **141**, 347 Trifluoroethanol

and water, internal dynamics of ranalexin: quantitative measurement of longitudinal and transverse cross-relaxation rates, Malliavin *et al.*, **140**, 189

p-Trifluoromethylphenyl[1,2-¹³C₂]acetate

¹⁹F–¹³C distances, REDOR-determined, Schaefer, **137**, 272

Triose-phosphate isomerase

yeast, transverse relaxation-optimized gradient-enhanced triple-resonance NMR spectroscopy, Loria, Rance, and Palmer, **141**, 180

Triphenylsilane

CSA/DD cross-correlated relaxation measurements, comparison of 1D and 2D (unbiased) experimental methods for, Batta, Kövér, and Kowalewski, **136**, 37

Triple-quantum filter

for ¹H NMR imaging of residual dipolar couplings in crosslinked elastomers, Schneider, Demco, and Blümich, **140**, 432

Triple-quantum-filtered NMR

¹H and ²H homonuclear and heteronuclear, dipolar interactions and dynamic processes of water in tendon, Eliav and Navon, **137**, 295

Triple-quantum-filtered twisted projection sodium MRI

human articular cartilage in vivo, Borthakur et al., 141, 286

Triple-resonance NMR

for correlation of H5 and exchangeable pyrimidine base hydrogens in ¹³C, ¹⁵N-labeled RNA, Wöhnert *et al.*, **139**, 430

multi-quantum HBHA(CBCACO)NH experiment with enhanced sensitivity for partially deuterated samples, Gschwind, Kessler, and Gemmecker, 137, 285

MUSIC: amino acid type-selective ¹H-¹⁵N correlations, Schubert *et al.*, **141**, 34

sensitivity-enhanced sim-CT HMQC PFG-HBHA(CO)NH and PFG-CBCA(CO)NH, Swapna and Montelione, 137, 437

3D ¹³C shift/¹H-¹⁵N coupling/¹⁵N shift solid-state NMR correlation spectroscopy, Gu and Opella, **138**, 193

transverse relaxation-optimized gradient-enhanced, Loria, Rance, and Palmer, **141**, 180

Triplet state

pentacene in *p*-terphenyl crystals, dynamic nuclear polarization in pulsed ENDOR, Kouskov *et al.*, **137**, 25

TROSY

comparison with S³ TPPI HSQC: suppression of heteronuclear coupling constants in multidimensional NMR, Schulte-Herbrüggen et al., 139, 443

gradient-enhanced triple-resonance NMR spectroscopy, Loria, Rance, and Palmer, 141, 180

measurement of ${}^1J_{\rm NC'}$ and ${}^2J_{\rm HNC'}$ couplings from spin-state-selective 2D correlation spectrum, Permi *et al.*, **140**, 32

multidimensional NMR experiments, design of, role of coherence-transfer efficiency, Meissner and Sørensen, 139, 439

pulse sequences for measurement of one-bond ¹⁵N-¹H coupling constants in protein backbone, Lerche *et al.*, **140**, 259

sensitivity improvement, Rance, Loria, and Palmer, 136, 92

suppression of diagonal peaks in TROSY-type ¹H NMR NOESY spectra of ¹⁵N-labeled proteins, Meissner and Sørensen, **140**, 499

three-dimensional HCCH, correlation of aromatic ¹H-¹³C groups in proteins, optimization, Meissner and Sørensen, **139**, 447

L-Tryptophan

¹H¹⁵N two-spin order in, decorrelation, detection of intermolecular chemical exchange through, Skrynnikov and Ernst, 137, 276

Tunneling

small tunneling splitting: spectroscopy from proton spin magnetization in rotating frame, Damyanovich, Peternelj, and Pintar, **140**, 9

Two-dimensional exchange NMR

dual processing of 2D exchange data in MAS NMR of solids, Tycko and Berger, 141, 141

⁸⁷Rb spin diffusion in ferroelectric RbH₂PO₄ studied by, Cereghetti and Kind, 138, 12

spectra, acquiring under slow MAS, Ernst, Kentgens, and Meier, ${\bf 138},\,{\bf 66}$ Two-dimensional NMR

2D $\{^{31}P\}$ spin-echo-difference constant-time $[^{13}C, ^{1}H]$ HMQC experiment for simultaneous determination of $^{3}J_{H3'P}$ and $^{3}J_{C4'P}$ in ^{13}C -labeled nucleic acids and protein complexes, Szyperski *et al.*, **140**, 491

¹⁹F, of oxyfluorides, high-order spin diffusion mechanisms in, Du, Levitt, and Grey, 140, 242

(HACACO)NH: J^{CH} -modulated pulse scheme for quantitative measurement of $^{13}C^{\alpha}-^{1}H^{\alpha}$ couplings in ^{15}N , ^{13}C -labeled proteins, Hitchens, McCallum, and Rule, **140**, 281

¹H/¹³C PISEMA experiments and application to backbone and side chain sites of amino acids and peptides, Gu and Opella, **140**, 340

high-temperature pulsed-field-gradient, of polymers, Liu *et al.*, **140**, 482 multiple-quantum, quadrupolar and chemical shift tensors characterized by, Medek and Frydman, **138**, 298

obtaining pure absorption 2D *J*-spectra, Mutzenhardt, Guenneau, and Canet, **141**, 312

solid-state, [1-15N]-2'-deoxyguanosine, magnitudes and orientations of 15N

chemical shift determined on polycrystalline sample by, Lorigan *et al.*, **140**, 315

suppression of systematic F_1 artifacts, randomized acquisition for, Bowyer, Swanson, and Morris, **140**, 513

Two-dimensional propagators

time correlations in fluid transport obtained by sequential rephasing gradient pulses, Stapf, Damion, and Packer, 137, 316

Two-dimensional spectra

simulations, pulsed-field gradients in, Meresi et al., 137, 186

Two-dimensional spectroscopy

accurate measurements of multiple-bond ¹³C-¹H coupling constants from phase-sensitive 2D INEPT spectra, Ding, **140**, 495

[15N, 1H] correlation spectrum, HN(α/β -COCA-J) experiment for measurement of $1J_{C'C^{\alpha}}$ couplings from, Permi et al., **141**, 44

phase-sensitive: composite PFGs with refocused chemical shifts and short recovery time, Hu and Shaka, 136, 54

protein hydration study using slaved pulses, Bornet, Guerlesquin, and Piotto, 138, 107

separation of ²H MAS NMR spectra, Kristensen et al., 139, 314

solid-state NMR, and selective and extensive 13 C labeling, in determination of multiple ϕ -torsion angles in proteins, Hong, **139**, 389

spin-state selective double-/zero-quantum 2D NMR spectra, measurement of homonuclear ²*J*-couplings from, Permi *et al.*, **139**, 273

triple-resonance experiments for correlation of H5 and exchangeable pyrimidine base hydrogens in ¹³C, ¹⁵N-labeled RNA, Wöhnert *et al.*, **139**, 430 unbiased, and 1D techniques, comparison for measurement of CSA/DD cross-correlated relaxation, Batta, Kövér, and Kowalewski, **136**, 37

Two-pulse phase-modulation (TPPM) decoupling

¹³C and ¹⁵N magic-angle turning with, resolution enhancement in, Mc-George, Alderman, and Grant, 137, 138

Tyrosyl radical

E. coli ribonucleotide reductase, pulsed ENDOR at 140 GHz, Bennati et al., 138, 232

U

Ubiquitin

measurement of homonuclear ²*J*-couplings from spin-state selective double-/zero-quantum 2D NMR spectra, Permi *et al.*, **139**, 273

 $^{15}N/^{13}C$ -labeled, measurement of $^1J_{\rm NC'}$ and $^2J_{\rm H^NC'}$ couplings from spin-state-selective 2D correlation spectrum, Permi *et al.*, **140**, 32

15N-labeled

excitation of selected proton signals, Pelupessy, Chiarparin, and Bodenhausen, 138, 178

identification of spin diffusion pathways in, Eykyn, Früh, and Bodenhausen, 138, 330

 3J (H_NH_{α}) couplings in, *J*-multiplied HSQC method for measurement of, Heikkinen *et al.*, **137**, 243

measurement of relaxation rates of $N^{\scriptscriptstyle H}$ and $H^{\scriptscriptstyle \alpha}$ backbone protons, Millet et al., 139, 434

off-resonance ROESY, tilt angle dependence of cross-relaxation in, Cutting, Ghose, and Bodenhausen, **138**, 326

offset profiles of selective pulses in, Eykyn, Ghose, and Bodenhausen, 136, 211

perdeuterated, observation of through-hydrogen-bond $^{2h}J_{\rm HC}$, Cordier *et al.*, **140**, 510

selective and extensive 13 C labeling, and 2D solid-state NMR, in determination of multiple ϕ -torsion angles in proteins, Hong, **139**, 389

٧

Vanadyl complexes

in glassy solution, spin-echo dephasing for, solvent and temperature dependence, Eaton and Eaton, 136, 63

Velocity selective perturbation

incorporation in RF pulse trains, Norris and Schwarzbauer, 137, 231

W

Wall relaxivity

and spin echo analysis of restricted diffusion under generalized gradient waveforms in porous media, Codd and Callaghan, 137, 358

Water

adsorption in zeolite 4A pellets, single-point MRI study, Prado, Balcom, and Jama, 137, 59

doped with triarylmethyl-based radical, ¹H DNP at 1.4 T, Wind and Ardenkjær-Larsen, **141**, 347

high-resolution NMR, suppression of radiation damping, Barjat, Mattiello, and Freeman, 136, 114

-protein interactions, editing of chemical exchange-relayed NOEs in NMR experiments for observation of, Melacini, Kaptein, and Boelens, 136, 214

state in gelatin gels, NMR relaxation study, Vackier, Hills, and Rutledge, 138, 36

in tendon, dipolar interactions and dynamic processes, ¹H and ²H homonuclear and heteronuclear MQF NMR study, Eliav and Navon, **137**, 295

and trifluoroethanol, internal dynamics of ranalexin: quantitative measurement of longitudinal and transverse cross-relaxation rates, Malliavin *et al.*, **140**, 189

Water diffusion

invariant and orthonormal scalar measures derived from MR diffusion tensor imaging, Bahn, 141, 68

measurements in brain, effects of local magnetic susceptibility-induced gradients in vivo, Clark, Barker, and Tofts, 141, 52

Water flipback

45°, signal enhancement using, for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

Water reference

artifacts introduced by zero-order phase correction in ¹H NMR and method of elimination by phase filtering, Wild, **137**, 430

Water suppression

signal enhancement using 45° water flipback for 3D ¹⁵N-edited ROESY and NOESY HMQC and HSQC, Gruschus and Ferretti, **140**, 451

Wavelet encoding

RF pulse design for, application: near-resonance solution to Bloch equations, Xu and Chan, 138, 225

W-hand

pulsed ENDOR spectrometer, setup and application to transition metal centers, Gromov et al., 139, 8

Χ

X-band EPR

at 10 K, large-magnitude high-spin nuclear parameters in Ti³⁺ center from, Tennant and Claridge, **137**, 122

129 X

in blood, T_1 and role of oxygenation, Albert *et al.*, **140**, 264 circulating laser-polarized, gas flow MRI using, Brunner *et al.*, **138**, 155 laser-polarized, single-shot diffusion measurement in, Peled *et al.*, **140**, 320 129 Xe $^{-1}$ H cross relaxation in aqueous solutions, consequences, Stith *et al.*, **139**, 225

¹³¹Xe

surface sensitive imaging of aerogels in liquid xenon near critical point, Pavlovskaya *et al.*, **137**, 258

X/1H filtering

suppression of ABX strong coupling signals in heteronuclear scalar and dipolar correlation spectra, Kövér and Batta, 138, 89

p-Xylene

–Dianin's inclusion compound, ¹³C distance measurements by 2D-RFDR, Zaborowski, Zimmermann, and Vega, 136, 47

Ζ

Zeolite 4A

pellets, water adsorption in, single-point MRI study, Prado, Balcom, and Jama, 137, 59

Zeolites

diffusion measurements in presence of internal gradients, PFGSE method for, Sørland, Aksnes, and Gjerdåker, 137, 397

Zirconium silicate

Ti³⁺ center in, large-magnitude high-spin nuclear parameters from X-band EPR at 10 K, Tennant and Claridge, **137**, 122

Statement of ownership, management, and circulation required by the Act of October 23, 1962, Section 4369, Title 39, United States Code: of

JOURNAL OF MAGNETIC RESONANCE

Published monthly by Academic Press, 6277 Sea Harbor Drive, Orlando, FL 32887-4900. Number of issues published annually: 12. Editor: Prof. Stanley J. Opella, Department of Chemistry, University of Pennsylvania, 231 South 34th Street, Philadelphia, PA 19104.

Owned by Academic Press, 525 B Street, Suite 1900, San Diego, CA 92101-4495. Known bondholders, mortgagees, and other security holders owning or holding 1 percent or more of total amount of bonds, mortgages, and other securities: None.

Paragraphs 2 and 3 include, in cases where the stockholder or security holder appears upon the books of the company as trustee or in any other fiduciary relation, the name of the person or corporation for whom such trustee is acting, also the statements in the two paragraphs show the affiant's full knowledge and belief as to the circumstances and conditions under which stockholders and security holders who do not appear upon the books of the company as trustees, hold stock and securities in a capacity other than that of a bona fide owner. Names and addresses of individuals who are stockholders of a corporation which itself is a stockholder or holder obods, mortgages, or other securities of the publishing corporation have been included in paragraphs 2 and 3 when the interests of such individuals are equivalent to I percent or proce of the total amount of the stock or securities of the publishing corporation have been included in paragraphs 2.

securities of the publishing corporation which resents a stockholder of holder of bonds, mortgages, or other securities of the publishing corporation have been included in paragraphs 2 and 3 when the interests of such individuals are equivalent to 1 percent or more of the total amount of the stock or securities of the publishing corporation. Total no. copies printed: average no. copies each issue during preceding 12 months: 1607; single issue nearest to filing date: 1675. Paid circulation (a) to term subscribers by mail, carrier delivery, or by other means: average no. copies each issue during preceding 12 months: 486, single issue nearest to filing date: 473. (b) Sales through agents, news dealers, or otherwise: average no. copies each issue during preceding 12 months: 68; single issue nearest to filing date: 68. (b) Outside the mail: average no. copies each issue during preceding 12 months: 27; single issue nearest to filing date: 27. Total no. of copies distributed: average no. copies each issue during preceding 12 months: 27; single issue nearest to filing date: 27. Total no. of copies distributed: average no. copies each issue during preceding 12 months: 1070; single issue nearest to filing date: 1031. Percent paid and/or requested circulation: average percent each issue during preceding 12 months: 91%; single issue nearest to filing date: 91%.

(Signed) Stephanie Smith, Asst. Manager, Journal Business Office