

GDCh-Fachgruppe Magnetische Resonanzspektroskopie
31ST DISCUSSION MEETING: Magnetic Resonance in Chemistry and Materials Research

Thursday, September 24, 2009

	A: Dynamics and Relaxation <i>S. Stapf</i>	H 4	B: EPR-methods <i>G. Jeschke</i>	403
08:30	D. Kruk (Bayreuth) NMR relaxation processes and dynamic properties of molecular systems		M. v. Gastel (Bonn) A theory for spin polarization effects and zero field splitting parameters in paramagnetic π -electron molecules and freeze-thawing chemical reactions by light: a progress report	
09:00	S. Klod (Dresden) ¹³ C NMR relaxation study of fullerenes: the influence of the nitride cluster in endohedral fullerenes		B. Endeward (Frankfurt) PELDOR spectroscopy on spin labeled RNA	
09:20	A. Herrmann (Bayreuth) Dynamics of polymer melts studied by fast field cycling 1H NMR		D. Hinderberger (Mainz) The structure and aggregation of myelin basic protein (MBP) in membranes and solution studied by EPR spectroscopy	
09:40	D. Reichert (Halle-Wittenberg) Direct observation of millisecond to second motions in proteins by dipolar CODEX NMR spectroscopy		E. Reijerse (Mühlheim) A quasi-optic high frequency pulsed/CW EPR spectrometer operating at 122 and 244 GHz	
10:10	<i>Coffee Break</i>			
	Low field NMR <i>B. Blümich</i>			H 4
10:40	P. Blümler (Juelich) Nested and hinged magnets for portable MRI, EPR and DNP			
11:10	G. Guthausen (Karlsruhe) Low field NMR in process monitoring and quality control			
11:30	M. Duewel (Mainz) Miniemulsion polymerization reactions observed by time-resolved xe-129 NMR			
11:50	N. Nestle (Ludwigshafen) Low-field NMR in industrial analytics and research: elastomer components, solution polymers, swelling and profiles			
12:20	Closing			

Tutorial
Monday, September 21, 2009

14:00-17:30	U. Scheler E. Brunner A. Vyalikh D. Reichert S. Stapf	405
13:00-14:30		
17:30-19:00	<i>Registration</i>	301
18:30-20:30	<i>Welcome</i>	304
19:00	Meeting of the GDCh Executive Committee Wenzel Prager Bierstuben, Königstr. 1	

Tuesday, September 22, 2009

08:30	Opening U. Scheler	
	Presentation of the Ernst-Awards <i>H. Kogler</i>	H 4
08:45	H. Kogler	
09:00	A. Marx (Darmstadt) Improved orientational properties of PBLG and PBDG	
09:20	Th. Rohmer (Leiden) Mas NMR study of the photoreceptor phytochrome	
09:40	<i>Coffee Break</i>	
	A: Inorganic materials <i>L. van Wüllen</i>	H 4
	B: Ligand interactions and drug design <i>W. Jahnke</i>	403
10:10	G. Buntkowsky (Darmstadt) Solid state NMR studies of nano-catalysts	Th. Peters (Lübeck) binding of (carbohydrate) ligands to native viruses and virus like particles
10:40	T. Echelmeyer (Münster) NMR- Investigations of Novel Solid State Lithium Ion Conductors	R. Stoll (Bochum) Dinuclear organo-iridium(III) mono- and bis-intercalators with rigid bridging ligands: synthesis, cytotoxicity and DNA binding
11:00	R. König (Berlin) AlFx(OR) _y -species identification in strongly disordered aluminium isopropoxide fluoride solids – a field dependent MAS NMR study	N. Lukzen (Novosibirsk, RU) Theoretical investigation of protein nmr saturation transfer to bioactive ligand
11:20	H. Eckert (Münster) NMR structural studies of paramagnetic nanocomposites	M. Vogtherr (Macclesfield, UK) Biomolecular NMR in pharmaceutical lead generation: Examples from AstraZeneca
11:50	<i>Lunch Break</i>	
12:30	Poster Discussion (odd numbers)	
	A: Polymers <i>U. Scheler</i>	H 4
	B: Metabolomics <i>H. R. Kalbitzer</i>	403
14:00	H. W. Spiess (Mainz) Solid-state NMR of functional materials	W. Kremer (Regensburg) 1H-NMR spectroscopy of blood plasma and cell cultures
14:30	F. Vaca Chavez (Halle) Polymer melt dynamics studied by low-field NMR	W. Gronwald (Regensburg) NMR and GC-MS based metabolomics
14:50	A. Karrasch (Berlin) Thermal decomposition of pdms in flame-retarded bisphenol-a polycarbonate: a solid-state NMR investigation	D. Leibfritz (Bremen) Analysis of Complex Lipid Mixtures by Combined Chromatography Methods, NMR Spectroscopy and Mass Spectrometry
15:10	M. R. Hansen (Mainz) Probing the assembly and dynamics of graphene-inspired molecular wires by solid-state NMR spectroscopy	
16:45	<i>Sightseeing</i>	
18:00	<i>Frauenkirche concert</i>	
19:30	<i>Dinner</i>	

Wednesday, September 23, 2009

	A: Solution NMR/Small molecules H 4 <i>E. Haupt</i>	B: Hybrid materials and biomineralizations 403 <i>E. Brunner</i>
08:30	N. Schlörer (Köln) Solution structure of chiral salen catalysts - conformational analysis assisted by paramagnetic NMR combining experiment and theory	Ch. Jäger (Berlin) Order and disorder in biominerals: News about bone and sea urchin spines
09:00	V. Schmidts (Darmstadt) Determination of conformer populations from residual dipolar couplings	Th. Köster (Münster) Coordination motifs of ions in polymer and composite electrolytes: A solid state NMR study
09:20	B. Fritzing (Ghent, B) Ligand interaction and dynamics in CdSe quantum dot dispersions: a solution NMR investigation	G. Brunklaus (Mainz) Investigation of local dynamics and structure in additive fortified epoxy resins via solid-state NMR
09:40	K. Karaghiosoff (München) Multinuclear NMR spectroscopy with small molecules	M. Bertmer (Leipzig) Solid-state NMR and EPR of magnetic coordination polymers based on Cu ₃ (BTC) ₂ and MIL-53
10:10	<i>Coffee Break</i>	
	A: Solution methods H 4 <i>Ch. Thiele</i>	B: Bio-Solids 403 <i>B. Reif</i>
10:40	B. Brutscher (Grenoble, F) Longitudinal-relaxation enhanced fast pulsing techniques: New tools for biomolecular NMR spectroscopy	C. Glaubitz (Frankfurt) Functional studies on membrane proteins by solid-state NMR and new methodological approaches
11:10	X. Yang (München) Numerically optimized INEPT sequence based on the optimal control theory and its experimental sensitivity enhancement for proteins with large transverse relaxation rates	G. Gröbner (Umeå,SE) Membranes as two-dimensional aggregation templates in amyloidogenic diseases: a biophysical solid state NMR approach
11:30	C. Liebold (Regensburg) Xenon-binding studies of the thermophilic enzyme HisF from <i>thermotoga maritima</i> using NMR-Spectroscopy	E. Brendler (Freiberg) 15N CP/MAS characterization of the nitrogen bonding situation in lignite based soil improving materials
11:50	M. Bennati (Göttingen) 1H and 13C Dynamic nuclear polarisation with a two-field (0.35/14 T) shuttle spectrometer	H. Heise (Düsseldorf, Jülich) Solid-state NMR spectroscopy of (paramagnetic) membrane proteins
12:20	<i>Lunch Break</i>	
13:00	Poster Discussion (even numbers)	

	A: Macromolecular structures H 4 <i>H. R. Kalbitzer</i>	B: Computational methods 403 <i>S. Glaser</i>
14:30	V. Dötsch (Frankfurt) Functional important dynamics in nonribosomal peptide synthetases	T. Ikeya (Frankfurt, Tokyo, JP) Protein structure determination in living cells by in-cell NMR spectroscopy
15:00	P. Kudla (Hamburg) Investigation of supramolecular structures in hair conditioners	M. Nimbalkar (München) Application of optimal control theory to NMR pulse sequence design
15:20	J. P. Klare (Osnabrück) Pulsed double electron-electron resonance (DEER) spectroscopy: A valuable tool for the study of protein function	J. Gimpler (Konstanz) Assignment optimization during protein structure calculation with a Max-Min Ant System
15:40	J. Balbach (Halle-Wittenberg) Functional protein folding intermediates studied by NMR spectroscopy	D. Sezer (Frankfurt) Toward quantitative analysis of dynamic nuclear polarization enhancements in liquids
16:10	<i>Coffee Break</i>	
	A: Solids Methods H 4 <i>E. Brunner/U. Scheler</i>	B: Imaging 403 <i>J. Bernarding</i>
16:40	A. Lange (Göttingen) Low-power solid-state NMR experiments for resonance assignment under fast magic-angle spinning	J. Braun (Berlin) Magnetic resonance elastography: in vivo rheometry of biological tissue
17:10	T. Bräuniger (Stuttgart) Signal enhancement of solid-state NMR spectra of quadrupolar nuclei with half-integer spin using SW-FAM pulse trains	F. Casanova (Aachen) NMR with small magnets
17:30	G. Hempel (Halle-Wittenberg) Investigations of the molecular structure of bent-core liquid crystals by 13C-1H and 1H-1H dipolar couplings	B. C. Dollmann (Mainz) Biocompatible, spin-labeled heparins as polarizing agents for dynamic nuclear polarization (DNP)
17:50	J. Schmedt auf der Günne (München) Quantitative lineshape analysis for 1D- and 2D-spectra of amorphous materials	J. Reichenbach (Jena) Susceptibility weighted imaging (SWI) principles and applications
18:30	Meeting GDCh members H 4	