BOOK OF ABSTRACTS

EURACT-NMR Workshop

January 27-29, 2010
Karlsruhe

Funded by the EU 7th Framework EURATOM Programme

CONTENTS

EURACT-NMR COMMITTEES 2
Local organizing committee 2
Members of the EU 7th Framework EU-NMR-An project "NMR expert round table" 2

GENERAL INFORMATION 3

BRUKER TOUR AND INE AND ITU VISITS 3

WORKSHOP DINNER 3

EURACT-NMR PROGRAMME 5

ABSTRACTS 7
P. Berthault 8
I. Furó 9
R. Kerssebaum 10
I. Fernández 11
C. Bessada 12
L.S. Natrajan 13
A. Ulrich 14
R. M. Gschwind 15
P. Kaden 16
J. Autschbach 17
R. Sarkar 18
G. Vidick 19
G. Pintacuda 20
A.J. Horsewill 21
C. Grey 22
R. E. Walstedt 23
A. Wong 24
S. Trumm 25
S. Kambe 26
C. Berthon 27
T. Charpentier 28

LIST OF PARTICIPANTS 29

EURACT-NMR committees

Local organizing committee

- Melissa A. DENECKE, KIT-INE, Germany
- Andreas GEIST, KIT-INE, Germany
- Joe SOMERS, JRC-ITU, Germany
- Anna SOCHA, JRC-ITU, Germany
- Natalie BRITSCHO, KIT-INE, Germany
- Frank BREHER, KIT-AC, Germany

Members of the EU 7th Framework EU-NMR-An project "NMR expert round table"

From left to right: Ian FARNAN (University of Cambridge, UK), Herman CHO, (Pacific Northwest Laboratories, USA), Jean F. DESREUX (University of Liège, BE), Daniel MEYER (CEA, FR), Andreas GEIST (KIT-INE, DE), Melissa A. DENECKE, (KIT-INE, DE), Zoltán SZABÓ (KTH, SE), Joe SOMERS (JRC-ITU, EU). Not shown, Frank Breher (KIT-AC, DE)

General Information

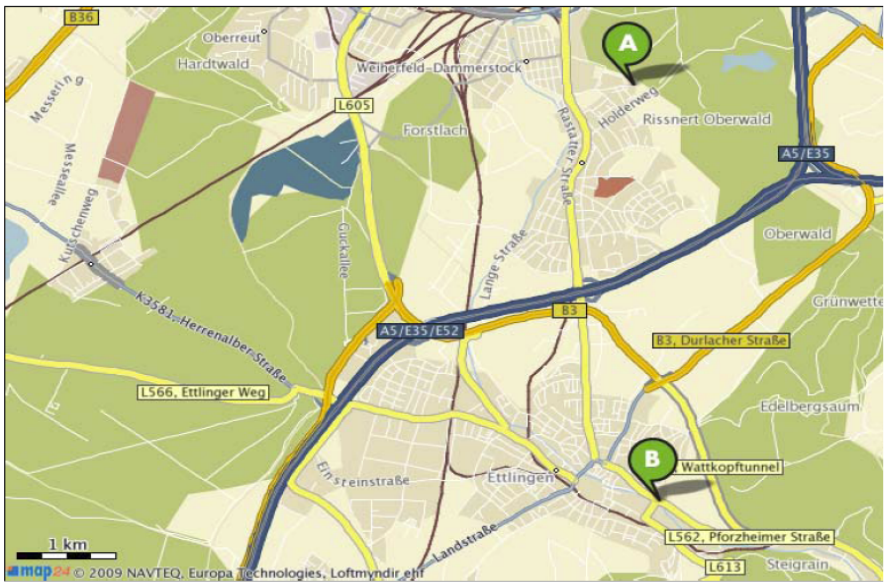
Welcome to EURACT-NMR Workshop at the Akademie Hotel Karlsruhe (Am Rüppurrer Schloss 40, 76199 Karlsruhe (Rüppurr). EURACT-NMR stands for "European Radioactive Nuclear Magnetic Resonance" and is aimed at establishing firm competence in Europe for NMR investigations of nuclear and radioactive materials. The workshop is being co-organized by the Karlsruhe Institute of Technology and the EU Joint Research Centre - Institute for Transuranium Elements (ITU), with scientific advice from other members of the NMR expert round table funded by the EU 7th Framework EURATOM Programme as a coordination and support action "EU-NMR-An – Towards a European Competence Centre for Nuclear Magnetic Resonance (NMR) on Actinides".

Bruker tour and INE and ITU visits

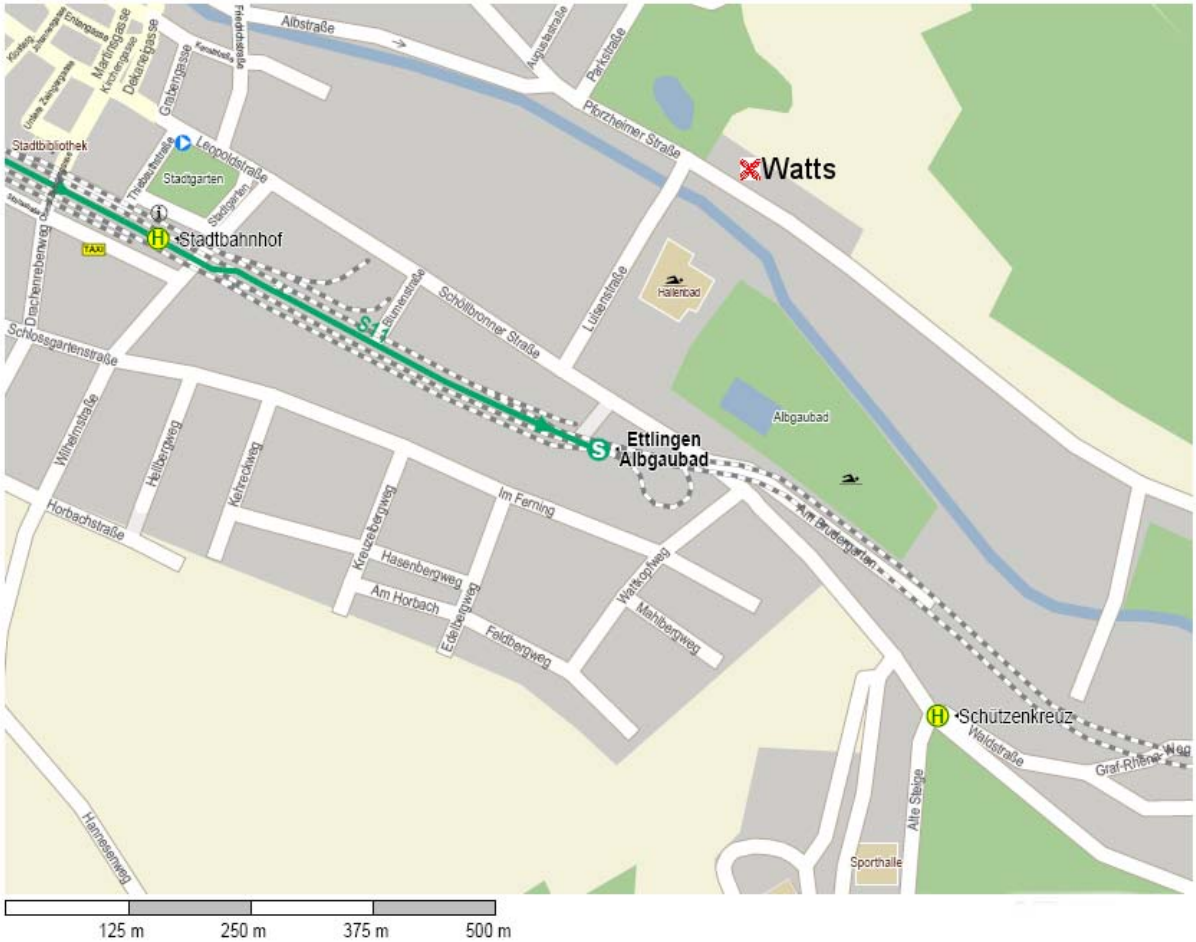
For those who have signed up at registration, there will be a tour of the Bruker BioSpin MRI facilities in Ettlingen on Thursday afternoon, 28. Jan. 2010. The bus will leave from in front of the hotel at 15:00.
The visits to KIT-INE and ITU are on Friday afternoon, 29. Jan 2010. The bus going to the KIT Campus North, where both institutes are located, will leave at 13:30 in front of the workshop hotel. The bus will return from ITU and KIT-INE to the workshop hotel. Departure is ca. 16:00.

Workshop dinner

The workshop dinner is on Thursday at 18:00 at Watts Brasserie (Pforzheimer Straße 67, 76275 Ettlingen). The participants of the Bruker BioSpin MRI tour will be transferred directly via bus. There is a bus organized to leave Bruker MRI at 17:30.
Those of you not participating in the Bruker tour must drive or use public transportation to the restaurant (tram S1 or S11 to Ettlingen-Albgaubad). It is easy to find (see maps).
All participants must take public transportation back from Watts to their respective hotels.



A=Akademie Hotel
B= Watts Brasserie


Albstraße
Augustastraße
Parkstraße
Pforzheimer Straße
Watts
Stadtbibliothek
Leopoldstraße
Stadtgarten
Stadtbahnhof
TAXI
Drachenreberweg
Schlossgartenstraße
Schöllbronner Straße
Blumenstraße
Luisenstraße
Hallenbad
Albgaubad
Ettlingen
Albgaubad
Wilhelmstraße
Heilbergweg
Kehreckweg
Horbachstraße
Kreuzelbergweg
Im Ferning
Hasenbergweg
Am Horbach
Edelbergweg
Feldbergweg
Wattkopfweg
Mahlbergweg
Am Brudergarten
Schützenkreuz
Waldstraße
Graf-Rhena-Weg
Alte Steige
Sporthalle
Hannesenweg
125 m
250 m
375 m
500 m

EURACT-NMR Programme

Wednesday, 27/01/2010

8:15 Registration

9:00 Greeting *(**Joe Somers**, ITU)*

9:10 Putting the nuclear back into nuclear magnetic resonance *(**Ian Farnan**, University of Cambridge)*

Modern NMR techniques and Methodology (Chair – Jean F. Desreaux):

9:30 Laser-Polarized xenon for NMR and MRI *(**Patrick Berthault**, CEA Saclay)*

10:15-10:45 Coffee Break

Hyphenated techniques:

10:45 Association of molecules and ions as observed by electrokinetic and diffusion NMR *(**István Furó**, Royal Institute of Technology)*

11:30 Increasing NMR sensitivity (***Rainer Kerssebaum***, *Bruker BioSpin GmbH*)

12:15 Lunch

Solution state NMR (Chair – Zoltán Szabó):

13:30 Unprecedented structures driven by the phosphinamide linkage – a multinuclear NMR touch ***(Ignacio Fernandez Nieves**, Universidad de Almería)*

14:15 NMR at high temperature in molten fluorides for nuclear applications: in situ experimental approach of the speciation *(**Catherine Bessada**, Université d'Orléans)*

15:00 Probing the solution speciation and coordination environment of f-element complexes by NMR and emission spectroscopy *(**Louise Natrajan**, University of Manchester)*

15:30-16:00 Coffee Break

NMR in organic chemistry and structural biology:

16:00 Solid state NMR of membrane-active peptides *(**Anne Ulrich**, Karlsruhe Institute of Technology)*

16:45 NMR on Organocopper Compounds *(**Ruth M. Gschwind**, Universität Regensburg)*

17:30 New developments for the measuring of RDCs *(**Peter Kaden**, KIT-INE)*

18:00 Posters + Get together with refreshments

Thursday, 28/01/2010

Solid state NMR (Chair – Ian Farnan):

9:15 Paramagnetic lanthanide labelling for NMR structure determination in the liquid and in the solid state ***(Guido Pintacuda**, Université de Lyon)*

10:00 NMR at cryogenic temperatures ***(Tony Horsewill**, University of Nottingham)*

10:45-11:15 Coffee Break

11:15 NMR studies of energy storage and related materials ***(Clare Grey**, University of Cambridge)*

Actinide/radionuclide NMR studies (Chair – Herman Cho):

12:00 Studies of actinide nuclear magnetism in actinide compounds ***(Russell E. Walstedt,** University of Michigan – Ann Arbor)*

12:45 Lunch

13:45 Slow MAS methodologies towards radioactive materials ***(Alan Wong**, CEA-Saclay)*

14:15 Towards understanding the An(III)/Ln(III) selectivity of BTP and BTBP N-donor extracting agents ***(Sascha Trumm,** KIT-INE)*

15:00 Departure visit to BRUKER Biospin GmbH, MRI division

ca. 18:00 Workshop Dinner, Watt's (Ettlingen)

Friday, 29/01/2010

Actinide/radionuclide NMR studies – *continued* (Chair – Herman Cho):

9:00 NMR study of exotic magnetism and superconductivity in actinide compounds ***(Shin Kambe**, Japan Atomic Energy Agency)*

9:45 NMR applied to liquid-liquid separation enhancement ***(Claude Berthon**, CEA Marcoule)*

10:30-11:00 Coffee Break

11:00 Structural studies of simplified nuclear waste glasses (***Thibault Charpentier,** CEA Saclay*)

11: 45 Lunch

13:00 Presentation of European NMR access ***(Daniel Meyer)*** and Closing panel discussion (Members of the EU-NMR-An round table)

13:30 Departure for Afternoon Lab tours (ITU + KIT-INE)

ca. 16:30 Lab tours end

Abstracts

LASER-POLARIZED XENON FOR NMR AND MRI

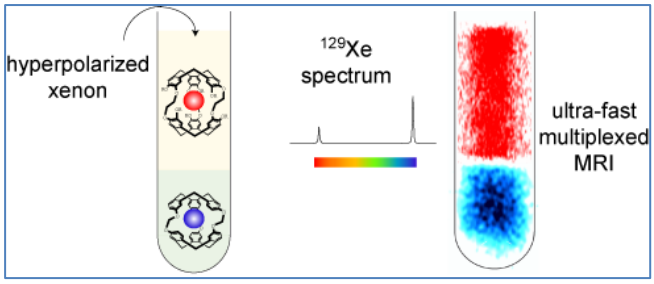
P. Berthault, C. Boutin, H. Desvaux, G. Huber, N. Tassali

CEA, IRAMIS, SIS2M, UMR CEA-CNRS 3299

Laboratoire Structure et Dynamique par Résonance Magnétique,

F-91191 Gif sur Yvette, France

NMR is widely recognized as a multiparametric technique for a detailed non invasive investigation of matter. However in some applications such as study of surfaces or biological cells, its lack of sensitivity limits its applicability. Developments improving either the polarization or the detection part can be undertaken to increase the NMR signal. Hyperpolarization techniques, which have been subjected to a renewal of interest these last years, can be sorted in three categories: DNP (Dynamic Nuclear Polarization), PHIP (ParaHydrogen Induced Polarization), and OP (Optical Pumping). We have chosen the last method to produce xenon with a nuclear polarization neighbouring 0.5 (Boltzmann polarization at 11.7 T multiplied by 45000). The deformability of the xenon electron cloud that gives it a pronounced hydrophobic character and a spectrum of wide chemical shift range induces that it is very sensitive to its local environment and therefore constitutes a powerful molecular probe. Our main activity leads in the conception of ^{129}Xe-NMR based biosensors where the noble gas is encapsulated in cage-molecules or nanoparticles functionalized with biological ligands [1]. The caged xenon having its own spectral signature opens access to a high-sensitivity spectroscopic imaging where a further gain in sensitivity is provided by the xenon in-out exchange, constantly renewing the host environment in hyperpolarization. Also we show that for hyperpolarized species, spin noise detection combined with inductively-coupled microcoils gives a further gain in sensitivity for samples of small volume [2].



Example of ^{129}Xe MRI where hyperpolarized xenon is detected in two different biosensors thanks to specific chemical shift of its caged form [3].

[1] P. Berthault, G. Huber, H. Desvaux, *Biosensing using laser-polarized xenon NMR/MRI*, Prog. NMR Spectrosc. **2009**, *55*, 35-60.

[2] H. Desvaux, D.J.Y. Marion, G. Huber and P. Berthault, *First nuclear spin-noise spectra of hyperpolarized systems,* Angew. Chem. **2009**, *121*, 4405-4407.

[3] P. Berthault, A. Bogaert-Buchmann, H. Desvaux, G. Huber and Y. Boulard, *Sensitivity and Multiplexing Capabilities of MRI Based on Polarized 129Xe Biosensors,* J. Am. Chem. Soc. **2008**, *130*, 16456-16457.

ASSOCIATION OF MOLECULES AND IONS AS OBSERVED BY ELECTROKINETIC AND DIFFUSION NMR

I. Furó, F. Hallberg, A. E. Frise, S. V. Dvinskikh, P. Stilbs

Division of Physical Chemistry and Industrial NMR Centre, Department of Chemistry

Royal Institute of Technology, SE-10044 Stockholm, Sweden

When ions, molecules, and particles associate, their characteristic translational mobility and their apparent charge change. Both of these properties can be accurately measured by two members of the family (or, rather, tribe) of NMR methods. One of those – diffusion NMR – has been with us for many years; some novel applications of it to ion pairing in ionic thermotropic liquid crystals will be mentioned [1]. The other technique – electrophoretic NMR or, perhaps in a broader sense, electrokinetic NMR (eNMR) – is not necessarily much younger but has remained less developed during the past decades. Methodological improvements [2] for eNMR experiments are presented with emphasis on improved signal-to-noise, accuracy, and accessibility and ease-of-use. The improved methodology is illustrated in applications to inclusion complexes [3] and ion pairing [4]. In a more applied direction, electrokinetic transport in fuel cell membranes will be assessed.

[1] A. E. Frise, T. Ichikawa, M. Yoshio, H. Ohno, S. V. Dvinskikh, T. Kato, and I. Furó, *Self-diffusion of ions in a confined nanostructure: NMR assessment of ionic conduction and ion pairing in a thermotropic liquid-crystalline bicontinuous cubic phase*, Chem. Commun., **2010**, *46*, in press.

[2] F. Hallberg, I. Furó, P. V. Yushmanov and P. Stilbs, *Sensitive and robust electrophoretic NMR. Instrumentation and experiments*, J. Magn. Reson. **2008**, *192*, 69-77.

[3] F. Hallberg, C. F. Weise, P. V. Yushmanov, E. Thyboll Pettersson, P. Stilbs and I. Furó, *Molecular complexation and binding studied by electrophoretic NMR spectroscopy*, J. Am. Chem. Soc. **2008**, *130*, 7550-7551.

[4] F. Hallberg, I. Furó and P. Stilbs, *Ion pairing in ethanol/water solution probed by electrophoretic and diffusion NMR*, J. Am. Chem. Soc. **2009**, *131*, 13900-13901.

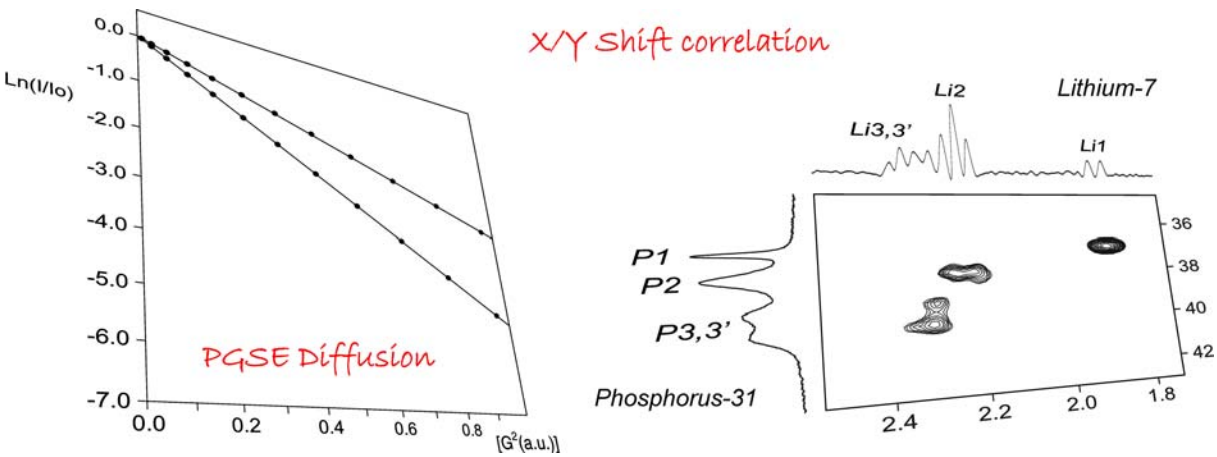
UNPRECEDENTED STRUCTURES DRIVEN BY THE PHOSPHINAMIDE LINKAGE – A MULTINUCLEAR NMR TOUCH

Ignacio Fernández

Área de Química Orgánica, Universidad de Almería, Ctra. Sacramento s/n, 04120, Almería, Spain.

Modern organic synthesis makes extensive use of organometallic compounds as intermediates species capable of performing carbon-carbon and/or carbon/heteratom bond-forming reactions with excellent chemo-, regio- and stereocontrol. In particular, organolithiums are the reagents most frequently used to achieve these transformations, where metalation usually depends on the directing power of a polar group present in the molecule that in fact contributes to the stabilization of a particular structure. Directed *ortho* metalation, D*o*M, has become a very powerful method for the preparation of substituted aromatic compounds. Recently, the phosphinamide linkage has shown to promote the *ortho* deprotonation of a *P*-phenyl ring very efficiently with high diastereo- or enantioselectivity, proving to be valuable intermediates for instance in the preparation of tin and gold complexes. Based on their synthetic potential we have been interested on the elucidation of their structures to help in the design of new goals in organic and coordination chemistry.

The examples presented herein illustrate the application of 1D NMR diffusion and 2D X/Y NMR correlation spectroscopy experiments on these studies. The former are commonly used to assist in determining the relative volume and then make a qualitative estimation of the amount of ion-pairing and/or state of aggregation. The latter allow one to detect directly the pattern of metal-ligand bonding interactions, or the connectivity between chemically significant heteroatoms in the molecular skeleton in cases where protons are absent, $^{n}J_{X,H}$ couplings vanish, or the coherence transfer via small long-range couplings becomes ineffective due to relaxation induced magnetization losses.



NMR AT HIGH TEMPERATURE IN MOLTEN FLUORIDES FOR NUCLEAR APPLICATIONS: IN SITU EXPERIMENTAL APPROACH OF THE SPECIATION

[1]**C. Bessada**, [2]A.-L. Rollet, [1]O. Pauvert, [1]A. Rakhmatullin, [1]V. Sarou-Kanian, [1]Mallory Gobet.

[1] CNRS, Université d'Orléans, UPR 3079 CEMHTI, 45071 Orléans, France;

[2] CNRS, UMPC - ESPCI, UMR 7195 PECSA, 75005 Paris, France.

The knowledge of the different ionic species existing in the melt, in terms of distribution, coordination and oxidation state is required for a better understanding of the physical and chemical properties of the molten salts. In electrolytic processes proposed for the pyrochemical treatments of spent nuclear fuel, the extraction efficiency is directly connected with the nature of ionic species existing in the reactive medium. The experimental difficulties inherent to such melts, and especially in the case of molten fluorides, have limited up to now any spectroscopic approaches. These liquids are corrosive, aggressive toward a number of materials, sensitive toward atmosphere and their melting temperatures are relatively high, compare to the commercial range covered usually by equipments. In the case of NMR, thanks to a laser heating system developed in our laboratory few years ago and associated with a closed boron nitride crucible, we are able to follow *in situ* the effect of the temperature or of the composition on the speciation in molten fluoride mixtures [1]. In order to characterize all the elements, because of the paramagnetism of the major part of lanthanides or actinides, we combine the NMR study of the anions (^{19}F; ^{17}O) and the cations (^{23}Na, ^{27}Al, ^{139}La, ^{91}Zr...) with EXAFS experiments (Zr, Th, U...). More recently, we have also developed a new device to measure self-diffusion coefficients at high temperature (up to 1300°C) in corrosive liquids. It is based on classical PFG NMR but coupled with the laser heating system. We have measured the self-diffusion coefficients of fluorine in different alkali and rare earth fluorides mixtures over a wide range of temperature and composition [2]. These measurements allow to describe different kinds of diffusion processes in relation with the structural description of such liquids: from a purely ionic liquid, with free ions in molten mixtures of alkali fluorides (LiF-NaF, LiF-KF, LiF-NaF-KF) where the dynamics is only governed by the temperature to network-like liquids (LiF-RF_3, R= rare earth) where the dynamics is governed by complexes formation.

These measurements open new perspectives in the study of high temperature liquids.

[1]C. Bessada, A. Rakhmatullin, A.-L. Rollet, D. Zanghi, *High temperature NMR approach of mixtures of rare earth and alkali fluorides: an insight into the local structure*, J. Fluor. Chem. **2009**, 130, 45-52.

[2]A.-L. Rollet, V. Sarou-Kanian, C. Bessada, *Measuring self-diffusion coefficients up to 1500K: a powerful tool to investigate the dynamics and the local structure of inorganic melts*, Inorg. Chem. **2009**, 48, 10972–10975.

PROBING THE SOLUTION SPECIATION AND COORDINATION ENVIRONMENT OF F-ELEMENT COMPLEXES BY NMR AND EMISSION SPECTROSCOPY

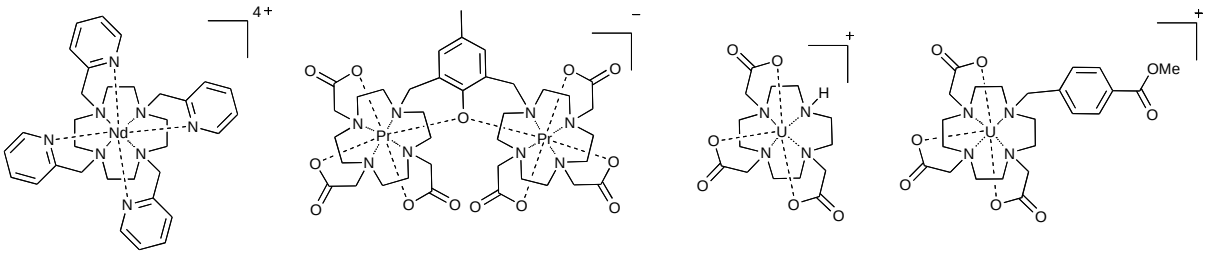
Louise S. Natrajan[a]*, Ntai M. Khoabane[b], Ilya Kuprov[b], Alan M. Kenwright[b] and Stephen Faulkner[a,c]

[a]School of Chemistry, University of Manchester, Oxford Rd., Manchester, M13 9PL, UK

[b] Department of Chemistry, University of Durham, South Rd., Durham, DH1 3LE, UK

[c] Chemistry Research Laboratory, University of Oxford, Mansfield Rd., Oxford, OX1 3TA, UK

Solution NMR spectroscopy is a powerful tool in determining structural properties of paramagnetic lanthanide compounds of DOTA[1] and its tetra-substituted derivatives provided the origin of the chemical shift is purely dipolar in nature. However, when the donor set anisotropy changes or when the symmetry deviates from an axial point group, NMR spectra become incredibly difficult to interpret and predict. In such cases, luminescence spectroscopy can be used as a complementary technique to elucidate the solution state structure and behaviour of lanthanide compounds. In the case of the actinides, the situation becomes further complicated due to the presence of a non-trivial contact contribution to the NMR spectral resonances. Despite this, a combination of NMR and emission spectroscopy can also prove informative in determining solution state behaviour. We will present a family of open shell lanthanide and uranium complexes derived from tetra and tri substituted cyclen derivatives and discuss their spectroscopic properties. To the best of our knowledge, these are the first U(IV) complexes that are emissive in solution at room temperature.



[1] S. Aime, M. Botta, G. Ermondi, *NMR Study of Solution Structures and Dynamics of Lanthanide(III) Complexes of DOTA*, Inorg. Chem., **1992**, *31*, 4291-4299.

SOLID STATE NMR OF MEMBRANE-ACTIVE PEPTIDES

Erik Strandberg, Parvesh Wadhwani, Sergiy Afonin, Stephan Grage, Jochen Bürck, Daniel Maisch, Christian Mink, Marco Ieronimo, **Anne Ulrich***

BioNMR group, IBG-2, Karlsruhe Institute of Technology,

*anne.ulrich@kit.edu

We are using solid state NMR to determine and compare the structures of various membrane-active peptides when bound to lipid bilayers. These include (a) antimicrobial peptides which kill bacteria by selectively permeabilizing their membranes, (b) cytotoxic peptides that are lytic also against eukaryotic cells, (c) cell penetrating peptides which can be used to carry cargo across membranes in a non-leaky fashion, and (d) fusogenic peptides that are able to merge two cells with one another. For highly sensitive ^{19}F-NMR structure analysis, the peptides are selectively labelled by attaching a single CF_3-group rigidly to the backbone in various different positions. Local orientational constraints are obtained by measuring the homonuclear dipolar couplings and chemical shift anisotropies of these labels in macroscopically oriented membrane samples. A set of several such constraints is then analyzed to yield the peptide conformation (e.g. α-helix, β-strand), its tilt angle and azimuthal rotation in the membrane plane, as well as its dynamic behaviour [1-4].

Since most of the peptides are secondary amphiphilic and cationic, it is not surprising that they all exhibit - at first sight - a similar tendency to bind as helices to the surface of (anionic) lipid bilayers and are further able to re-align into transmembrane pores. However - at a closer look - some of these sequences differ fundamentally in their response to, for example, changes in the lipid phase state or the type of acyl chains encountered. More subtle effects are observed when comparing how the respective re-alignment equilibria depend on the peptide concentration or the type of lipid head group. Altogether, these NMR studies with selectively labelled peptides serve to illustrate that it is possible not only to characterize their conformation and orientation, but also to observe fast and low exchange between different states, to describe the extent of molecular wobble, and to infer the degree of peptide oligomerization and/or aggregation. All these properties need to be collected and considered in an attempt to derive some general principles by which the activity of any designer-made peptide can be optimized that is supposed to carry out one specific pharmaceutical function.

[1] D. Maisch, P. Wadhwani, S. Afonin, C. Böttcher, B. Koksch, A.S. Ulrich (2009) JACS, 131: 15596

[2] E. Strandberg, S. Esteban-Martin, J. Salgado, A.S. Ulrich (2009) Biophys. J., 96: 3223

[3] P. Wadhwani, J. Buerck, E. Strandberg, C. Mink, S. Afonin, A.S. Ulrich (2008) JACS, 130: 16515

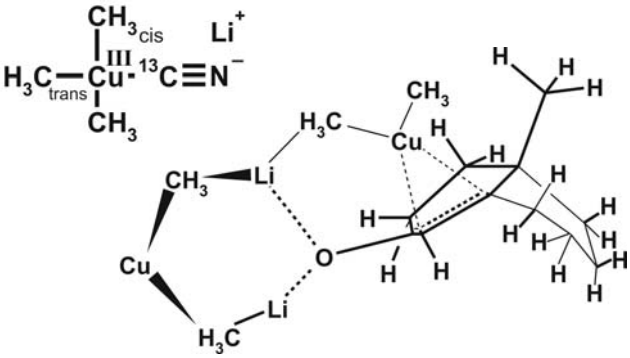
[4] S. Afonin, S.L. Grage, M. Ieronimo, P. Wadhwani, A.S. Ulrich (2008) JACS, 130(49): 16512

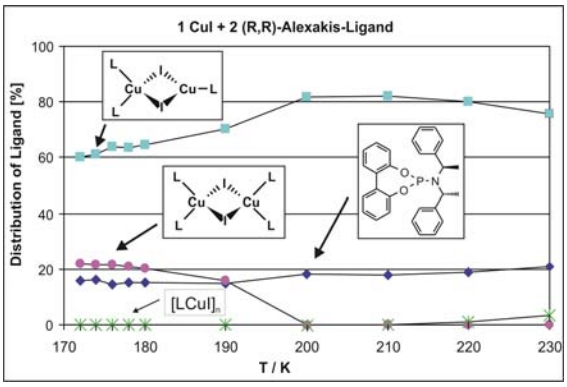
NMR ON ORGANOCOPPER COMPOUNDS

R. M. Gschwind

Institute of Organic Chemistry, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany

A key role of organometallic reagents and catalysts is generally accepted in various fields of organic and inorganic synthesis. However, the structure elucidation of organometallic compounds by NMR in solution is often hampered by highly symmetrical, sometimes supramolecularly aggregated structures, especially in the case of metals with large quadrupole moments and structures which show dynamic equilibria between several species and which are sensitive to solvent and salt effects. On famous organocopper compounds a stepwise NMR approach for the structure elucidation of organocopper compounds in solution is presented.[1] Actual examples are dimethylcuprates as generally accepted mechanistic model system for organocopper reagents and phosphoramidite copper complexes as one of the most famous catalytic systems used in synthesis. As highlights e.g. Cu(I) and Cu(III) intermediates of organocuprates [2, 3] and the temperature dependent interconversion of catalytically active phosphoramidite copper complexes [4] (see Figure) are presented.





[1] R. M. Gschwind, *Organocuprates and Diamagnetic Copper Complexes: Structures and NMR Spectroscopic Structure Elucidation in Solution*, Chem. Rev., **2008**, *108*, 3029-3053.

[2] W. Henze, T. Gärtner, R. M. Gschwind, *Organocuprate Conjugate Addition: The Structural Features of Diastereomeric and Supramolecular π-Intermediates,* J. Am. Chem. Soc., **2008**, *130*, 13718-13726.

[3] T. Gärtner, W. Henze, R. M. Gschwind, *NMR-Detection of Cu(III) Intermediates in Substitution Reactions of Alkyl Halides with Gilman Cuprates,* J. Am. Chem. Soc., **2007**, *129*, 11362-11363.

[4] K. Schober, H. Zhang, R. M. Gschwind, *Temperature-Dependent Interconversion of Phosphoramidite-Cu Complexes Detected by Combined Diffusion Studies, ^{31}P NMR, and Low-Temperature NMR Spectroscopy,* J. Am. Chem. Soc., **2008**, *130*, 12310-12317.

NEW DEVELOPMENTS FOR THE MEASURMENT OF RDCS

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Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

In recent years NMR spectroscopy in anisotropic environment has evolved into an integral part of the process of structure determination and the analysis of the dynamics of molecules in solution. The facile access to measured data is a large improvement in structure elucidation. Information on the location vector relative to the magnetic field can easily be extracted from the directional dependence of the residual dipolar couplings. This allows for addressing questions that could not be answered by a narrow network of NOE data. Foundation of these investigations is an appropriate orienting medium which possesses a sufficiently low orienting ability. The identification of an adequate orienting medium, which should be specifically suited for the individual research project, is essential.

Only in the last decade, orienting media for the use with organic solvents were developed. Essential for the usage as orienting medium in this area is the facile scalability of the orienting properties (e.g. stretching of swollen gels). Two newly developed gels, namely polymethylmeth-acrylate and polyurethane gels, are presented. Examining the results of the swelling experiments concerning the resulting deuterium splitting of the solvent, one observes initially a non-trivial curve behavior. A modification of the theory of Kuhn and Grün accounts for the uniaxial swelling of the gels and leads to a new linear correlation of the observed deuterium splitting to the elastomer properties of the gels. This results in a better understanding of the material properties and additionally provides an easily determinable parameter, which correlates linearly along the shown equations with the orienting strength of the medium.

The determination of the residual dipolar couplings is often hampered by huge residual signals of the polymer or of residual monomers. Due to overlap of groups of signals in the measured spectra coupling constants cannot be determined with the necessary accuracy. Methods suppressing unwanted signals of the polymer by isotope labeling and subsequent application of suitable filtering methods are often not applicable. It is demonstrated that the signals of the polymers are easily distinguished by the differences of their physical properties. A filtering motif using the different diffusion properties of polymers and the solute molecules is successfully established for the identification and elimination of the signals of the polymer.

COMPUTING NMR PARAMETERS OF HEAVY ELEMENTS SYSTEMS USING DENSITY FUNCTIONAL THEORY

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We will discuss relativistic density functional theory (DFT) based methods that can be used for the calculation of NMR parameters in heavy-element systems, and discuss a number of illustrative applications. The use of a relativistic theory is important for molecules with heavy nuclei. The focus will be on the efficient ZORA method to treat relativistic effects. The computational strategy depends on the system of interest. For example, for light atomic ligand NMR properties both pseudopotentials and direct all-electron methods can be applied. For NMR parameters of heavy nuclei themselves, direct methods are preferred. Relativistic "corrections" to magnetic resonance parameters of heavy elements can amount to hundred per cent of a nonrelativistic result, or more (in particular for J-coupling). Spin-orbit coupling can strongly influence chemical shifts of heavy nuclei as well as of light nuclei in their vicinity, and may impact J-coupling between heavy p-block elements. Heavy-element hyperfine integrals should be caluclated with a finite-nucleus model. We will specifically demonstrate the importance of modeling solvent effects when a comparison is to be made between computed NMR parameters with experimental data obtained from solution. We will briefly discuss the calculation of NMR chemical shifts in molecules and metal complexes with unpaired electrons.

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COMPLEX INTERPLAY OF Ce-4F AND Fe -3D MAGNETISM IN CeFe(As,P)O AS SEEN FROM ^{31}P AND ^{75}AS NMR.

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The rare earth (R) transition metal (T) pnictides RTPnO(Pn:P orAs) earn special attention because of the high T_C superconductivity in $CeFeAsO_{1-x}F_x$, whereas the magnetism of the undoped system stays unexplored. CeFePO is a heavy fermion metal with a high γ value (700 mJ/mol K^2) in the vicinity of aferromagnetic (FM) instability [1]. Here magnetism is solely governed by Ce-4f state whereas in CeFeAsO, Fe-3d states themselves order AFM at about T $\cong$ 150 K. Therefore investigation on CeFe(As,P)O allows to study the crossover between Kondo and RKKY physics to 3d magnetic order. Yongkang Luo et. al.[2] recently published a rather complex phase diagram with two critical points obtained from bulk properties. NMR provides a microscopic tool for studying the interplay between Ce - 4f and Fe - 3d magnetism. We report on ^{31}P (I=1/2) and ^{75}As (I=3/2) NMR studies on $CeFeAs_{1-x}P_xO$ with x=0, 0.05, 0.3, and 0.9.

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[2]. Luo et . al. arXiv:0907.2961v1.

AN NMR INVESTIGATION OF THE ACTINIDE IONS AND THEIR COMPLEXES

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We currently use several advanced NMR techniques in order to fully characterize actinide ions and their complexes in water or in organic solvents. The dispersion of the longitudinal relaxation time T_1 of solvent nuclei with the magnetic field (NMRD) yields information on the magnetic properties and on the dynamic behavior of paramagnetic species. ^{17}O NMR allows the measurement of the water exchange times and ^{1}H and ^{13}C spectra yield information on the solution structures of the complexes and on the covalency of their coordination bonds. The application of NMR in actinide science will be illustrated with studies on the U, Np, Pu and Cm ions in different oxidation states and on their complexes.

For instance, Cm^{3+} is the actinide analogue of Gd^{3+} but is not in a pure ^{8}S state as indicated by much lower relaxation rates and much shortened electronic relaxation rates. In keeping with EPR studies[1], Cm^{3+} does not have a perfectly spherical distribution of its unpaired electronic spins because of a much stronger spin-orbit coupling. Moreover, the Cm^{3+} relaxivity originates from three different processes: a dipolar coupling between the nuclear and electronic spins, a delocalization of unpaired electronic spins into the solvent orbitals (contact interaction) and a Curie contribution. Each process gives rise to an inflection point in the NMRD curves and the contact interaction reflects the partial covalency of the coordination bonds formed by Cm^{3+}. A contact contribution is also observed in the NMR spectra of Cm^{3+} complexes.

The sensitivity of NMR to the exact nature of the ground state of actinide ions is also illustrated by detailed studies on the U, Np and Pu ions in different oxidation states. For instance, a comparison of the NMRD curves of the $5f^2$ ions U^{4+}, NpO_2^{+} and PuO_2^{2+} indicates that the two dioxo cations have abnormally long electronic relaxation times. However, well-resolved ^{1}H NMR spectra of their complexes can be obtained provided the solution species are sufficiently rigid. It will be shown that NpO_2^{+} and PuO_2^{2+} induce dipolar paramagnetic shifts from which the solution structure can be deduced.

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PARAMAGNETIC LANTHANIDE LABELLING FOR NMR STRUCTURE DETERMINATION IN THE LIQUID AND IN THE SOLID STATE

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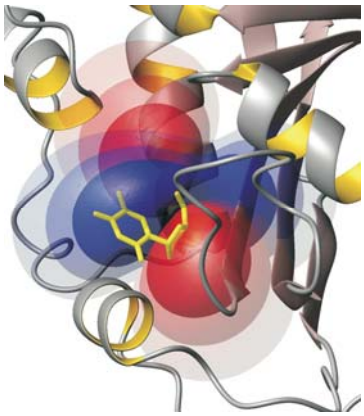
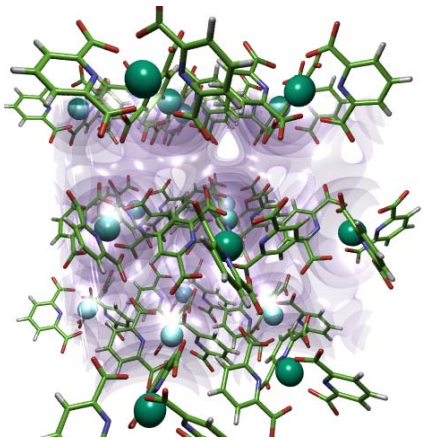
The paramagnetism of lanthanide ions offers outstanding opportunities for fast determinations of the three-dimensional (3D) structures of protein-protein and protein-ligand complexes and of inorganic materials by nuclear magnetic resonance (NMR) spectroscopy.

First, we review the potential of lanthanide ions in biomolecular liquid-state NMR. It is shown how the combination of pseudocontact shifts (PCS) induced by a site-specifically bound lanthanide ion and prior knowledge of the 3D structure of the lanthanide-labeled protein can be used to achieve (i) rapid assignments of NMR spectra, (ii) structure determinations of protein-protein complexes, and (iii) identification of the binding mode of low-molecular weight compounds in complexes with proteins. [1]

Second, we illustrate a protocol that uses the effects originating from paramagnetic lanthanide ion for structure determination of powdered microcrystalline complexes at natural isotopic abundance. The protocol makes use of paramagnetic effects, measured on suitably recorded ^{1}H MAS NMR spectra, to simultaneously define the conformation of a molecule in the lattice and the intermolecular packing in the solid phase. [2]





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NMR AT CRYOGENIC TEMPERATURES

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Performing NMR at low temperatures has many potential advantages, not least of which is the substantial increase in NMR signal intensity that accrues. One of the biggest limitations of the NMR technique is its poor inherent sensitivity so given the NMR signal increases as the inverse temperature there is increasing interest in performing experiments in a cryogenic environment. However, the instrumentation and NMR properties in this environment can pose significant challenges. In this talk a range of Cryogenic NMR experiments will be discussed to illustrate some of applications that contribute to our understanding of important processes in the physical sciences, particularly in the field of molecular motion, together with some technological solutions.

OPTIMIZING MATERIALS FOR BATTERY AND ENVIRONMENTAL APPLICATIONS: APPLICATION OF NMR TO PARAMAGNETIC MATERIALS

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The development of the lithium-ion battery has enabled many of the modern electronics that increasingly form an integral part of society in the 21st century. The $LiCoO_2$/graphite cell commercialized by SONY in 1990, while adequate for many low power applications, will not meet all the requirements for high power devices. The high power applications include hybrid electric vehicles (HEVs) and electric vehicles (EV), the current vehicles using nickel metal hydride (and lead-acid) batteries. Cheaper, safer batteries, which can be charged and discharged faster, last longer and can withstand a wide range of temperatures, are required to power these devices. Our work has focused on an understanding of the role that local structure plays in controlling electrochemical function. For example, ^{6}Li MAS NMR spectroscopy has been used to study local electronic structures and Li local environments in a variety of potential cathode materials for lithium ion batteries including spinels and layered cathode materials such as $Li[M'_xM_{1-x}]O_2$ (M,M' = Mn, Ni, Co *etc*.). We first developed a fundamental understanding of the causes of the large (hyperfine) NMR shifts typically observed in these paramagnetic samples. This knowledge was then applied, to follow structural changes after charging and discharging of a battery, to help establish why some materials function well as electrode materials and others fail.

The second part of the talk will describe the development of methods for examining Fe-containing paramagnetic minerals, by using NMR spectroscopy. The work has focused on the iron oxyhydroxides often found in soil samples, these oxides representing important sorbates for toxic ions such as Pb^{2+} or $H_2AsO_4^-$. By tuning the magnetic properties of the materials (where necessary), we can obtain high-resolution NMR spectra of common iron-containing soil minerals such as goethite, lepidocrocite and akaganeite, for the first time. This has allowed us to monitor ion binding and defect structures under environmentally-relevant conditions. For example, we have shown that Li^+ ions form inner-sphere complexes on goethite and lepidocrocite surfaces at low relative humidities, and outer-sphere complexes at higher humidities. We have used ^{31}P MAS NMR to distinguish between surface-bound species and the formation of iron phosphate precipitates, via dissolution-precipitation mechanisms.

STUDIES OF ACTINIDE NUCLEAR MAGNETISM IN ACTINIDE COMPOUNDS

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NMR studies of actinide compounds will be reviewed, with an emphasis on determination of the NMR shifts or local hyperfine (HF) fields, quadrupolar splittings, and/or spin-lattice relaxation times of the actinide nuclei themselves. Actinide nuclear spin magnetism reflects the behavior of the 5f electrons in a very direct way, offering strong motivation to tap into the corresponding NMR parameters. The survey planned will include three experimental scenarios for measurement of actinide nuclear spin behavior, with a brief summary of relevant data for each from work performed by the *Uranium NMR Group* at the Advanced Science Research Center of the Japan Atomic Energy Agency in Tokai-mura, Ibaraki Prefecture, Japan, where I was group leader from 2000 – 2005 [1]. The principal topics of the talk will include direct observation of ^{235}U pulsed NMR in antiferromagnetically ordered systems [2], indirect measurement of T_1 for ^{235}U in a metallic environment [3], and indirect measurement of T_1 and T_2 for ^{237}Np in NpO_2 and other systems [4]. In all of these systems ligand NMR was also observed either as a means to obtain the actinide results or as a supplement to them. Based on these examples, studies of actinide nuclear magnetism are suggested to be feasible in a wide range of related compounds.

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SLOW MAS METHODOLOGIES TOWARDS TO RADIOACTIVE MATERIALS

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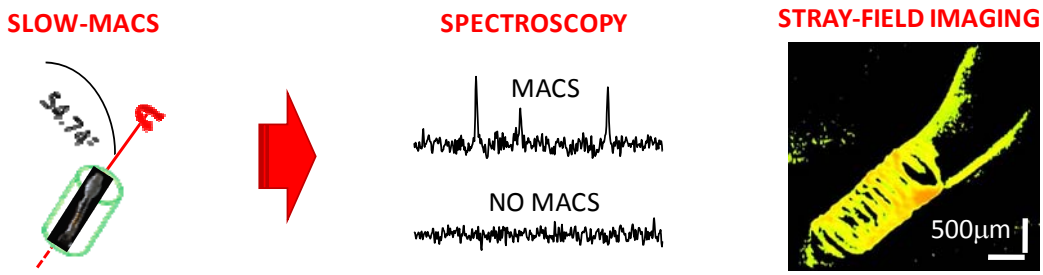
In the past two decades, solid-state NMR has become an indispensable analytical tool for studying crystalline and amorphous materials such as silicates, zeolites, concretes and glasses. However, not until recently MAS studies on radioactive solids were applied.[1] This is due to the challenges of handling radio-toxic materials, where sample preparations and characterizations, including MAS measurements, must be performed with extreme caution. Well-designed experimental protocols must be implemented to ensure absolute safety. Here, we propose MAS strategies that may offer high-resolution spectroscopy and imaging with safety enhancements. These could potentially be adoptable for studying radioactive samples: (1) high-sensitivity MAS measurements of micro-sized (MACS) samples[2,3] to prevent handling large quantities of hazardous materials; (2) ultra-slow MAS experiments for enhancing safety of the spinning, especially for samples with fission products; (3) NMR measurements from a small portable magnet could indeed lessen the experimental challenges and enhance safety. We will present experimental results of slow MAS high-resolution spectrsocopy[3,4] and imaging of micro-sized samples, and an approach to magnet design that can give arbitrary magnetic fields using permanent magnets.[5] The above three approaches could, in principle, be applied in the case of a magnetic field rotating at the magic angle. This is certainly a difficult task, but possibly attainable with the knowledge acquired from the above individual works. However, this would enhance the safety and alleviate the difficulties of performing high-resolution spectroscopy and imaging for the chemical analysis of radioactive materials.



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TOWARDS UNDERSTANDING THE AN(III)/LN(III) SELECTIVITY OF BTP AND BTBP N-DONOR EXTRACTING AGENTS

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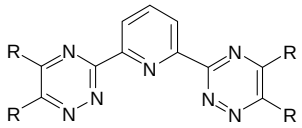
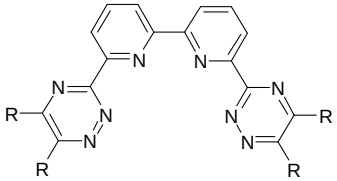
The Partitioning & Transmutation strategy aims at minimising used nuclear fuel's long-term radiotoxicity, by separating actinides (U, Np, Pu, Am, Cm) and re-using them as nuclear fuel. Due to their chemical similarity, the separation of trivalent actinides [Am(III), Cm(III)] from the lanthanides is a key step. This separation is only possible using extractants bonding via soft donor atoms (such as N or S). A breakthrough in this field was the development of alkylated BTPs at INE [1].Later, tetradentate alkylated BTBPs were developed from the BTPs, with $CyMe_4$-BTBP [2] being the current reference extracting agent for process development in Europe.



BTP



BTBP

We perform fundamental investigations aimed at understanding the driving forces of BTPs' and BTBPs' selectivity. To this, we investigate and compare structure and speciation of trivalent actinides and lanthanides complexed with BTP or BTBP in solution. EXAFS studies [3, 4] reveal similar structures of $[M(III)(BTP)_3]^{3+}$ (M = U, Pu, Am, Cm, Eu, Gd) complexes in solution. On the other hand, TRLFS speciation studies [3, 4, 5] show that the extractable BTP and BTBP complexes form at much lower ligand concentration with Cm(III) as compared to Eu(III).

We start implementing NMR as a novel technique for studying such systems. As these investigations involve actinide complexes they are only feasible with the appropriate infrastructure as is the case in KIT-INE's NMR lab which is currently being installed.

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NMR STUDY OF EXOTIC MAGNETISM AND SUPERCONDUCTIVITY IN ACTINIDE COMPOUNDS

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Advanced Science Research Center, Japan Atomic Energy Agency

In the condensed matter physics of strongly correlated electron systems, actinide (5f) compounds are regarded as the last unexplored field which shows many exciting phenomena such as unconventional superconductivity and multi-polar magnetic ordering. For example, the first Np-based unconventional superconductor $NpPd_5Al_2$ was discovered in 2007. Furthermore, among actinide dioxide systems AnO_2, NpO_2 shows octupolar magnetic ordering for the first time, whereas the ground ordered state of AmO_2 has not yet been identified. NMR is quite an effective method for clarifying the nature of magnetism and superconductivity, since it can probe low-energy static and dynamic properties of spins (by NMR) and charges (by NQR). In addition to electronic properties, NMR is also useful for a characterization of defects in *e.g.* actinide dioxides, which is important for development of high performance MOX nuclear fuel.

In my talk, I would like to discuss ways that NMR is powerful in this field, review our recent NMR studies in actinides compounds such as $NpPd_5Al_2$ and AnO_2, and finally, give a perspective on other research topics in this field.

INTEREST OF NMR IN THE FIELD OF RADIOACTIVE ENVIRONMENTS EXAMPLES AND LIMITS

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To support liquid-liquid extraction applied to fuel reprocessing, two 400MHz NMR spectrometers are available in our team (DRCP/SCPS/LILA). Both are kitted out with direct and reverse gradient 5mm probes and 4mm or 7mm CP/MAS probes. One of them is especially dedicated to radioactive samples.

Studies we mainly deal with, involve liquid state samples and from time to time radioactive materials. Experiment studies of solutions are wide. It can be merely quantitative measurements like TBP radiolysis study, characterization of organic or aqueous phase species with lanthanide or actinide cations, diffusion coefficient measurements to look at extractant aggregations like malonamides, reach concentration profiles as close as possible to the liquid-liquid interface through a localized NMR spectroscopy (M. Bardet collaboration), conformational studies of metallic species formed in solutions by using paramagnetic cations as a probe, etc. More fundamental researches about paramagnetic behavior of actinide ions in solutions are under study, for a better understanding of the 5f electrons (PhD student S JAN and collaboration with JF Desreux).

Glove boxes available in our laboratory allow any kind of radioactive experiments with α radioisotopes in solutions and at different temperatures. However, radioactivity of elements like Am(III) or Cm(III) is too high and need to be handled with low concentration samples. So, encountered difficulties to study such radioactive samples through NMR spectroscopy are not due to confinement or safety experimental reasons but rather sensitivity to get good spectra. With our standard experimental NMR facilities, ^{13}C NMR spectra can not be obtained for sample concentration below 10^{-2}M. To overcome this limit, it would be useful to get cryogenically cooled probes.

Solid state experiments carried out in the laboratory only deal with radioactive samples like Pu-doped glass or contaminated ashes with T. Charpentier help. Information we look for (quantitative measurements or characterisation of sites) need usually high resolution spectra. Unlike liquid state sample NMR experiments, experimental difficulties arise from safety reasons because of the high spinning speed of the rotors. To overcome this, two ways are under study in the laboratory: one based on 2D NMR pulse sequences designed for low spinning speed and one base on the narrow bore CP/MAS probe head nuclearisation.

STRUCTURAL STUDIES OF SIMPLIFIED NUCLEAR WASTE GLASSES

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Solid state NMR has now become a well established tool for the structural characterization of a wide class of crystalline and amorphous materials. In these respects, glassy materials have greatly benefited from the increasing level of sophistication of NMR experiments and processing. We will present how recent advances in NMR provide detailed structural information on the local environment of atoms in glasses, such as bond angle distributions, charge-compensation mechanisms, distribution of alkali and alkali-earth cations, in correlation with the glass composition. It will be shown how the recent introduction of first-principles calculations of NMR parameters combined with Molecular Dynamics simulations yields a very promising quantitative support of the NMR experiments [1]. Structural studies of inactive simplified nuclear waste glasses modelling the French nuclear glass (structure, surface alteration, irradiation effects) will be presented as an illustration of the present state-of-the-art of those high-resolution solid-state NMR methodologies [2].

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