




# April 15 – 20, 2012

## INTERCONTINENTAL HOTEL MIAMI

### Miami, Florida

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## POSTERS

All posters should be set up 8:00 to 9:00 am on Monday and removed at 3:45 pm on Thursday. Be sure to use the poster space number printed here. Authors of odd-numbered posters present on Monday and Wednesday. Even numbered posters present on Tuesday and Thursday.

**Luis Fernando Cabeca**; Luiza Maria da Silva Nunes; Paulo Falco Cobra; Luiz Alberto Colnago; *EMBRAPA Instrumentation, São Carlos, Brazil*

The combination of electrochemical (EC) and Nuclear Magnetic Resonance (NMR) has been rarely performed due to distortion of the static magnetic field ( $B_0$ ) homogeneity. Because of the bench top NMR (Time Domain – TDNMR) low homogeneity, the distortion caused in magnetic field by the electrodes is not critical. Therefore, the copper electrodeposition reaction can be monitored using the Carr-Purcell-Meiboom-Gill (CPMG) to measure transverse relaxation time. The results showed that  $\text{Cu}^{+2}$  concentration decreased rapidly with the electrodeposition until 100 min, and then, remained constant. After 3 hours reaction the  $\text{Cu}^{+2}$  concentration was  $2 \times 10^{-3}$  M, corresponding to 10% of the initial  $\text{Cu}^{+2}$  concentration. The measures show that EC-TDNMR combination can be very fast, simple and an efficient technique to monitor electrodeposition reaction.

Poster 121

### Multiple Spin Coherences and the Time Evolution of a Magic Echo

**Steven Morgan**<sup>1</sup>; Vadim Oganessian<sup>2</sup>; Gregory Boutis<sup>1</sup>; <sup>1</sup>Brooklyn College/CUNY, Brooklyn, NY; <sup>2</sup>College of Staten Island/CUNY, Staten Island, NY

We report on an average Hamiltonian treatment of a magic echo to second order. The degradation of time-reversal with increasing evolution time is shown theoretically and via simulation and experiment to be strongly influenced by finite pulse width effects. We investigate the spin dynamics under a magic echo sequence beyond the single-spin, single-quantum portion of the density matrix. In a sample of adamantane we observe that the evolution of multiple spin correlations following a magic echo is similar to the FID even though the overall signal amplitude decreased more than 50% for the longest magic echo measured. Additionally, the long-time portion of the coherences detected is observed to decay at the same rate for both the FID and magic echoes.

Poster 122

### Methodology to Measure Temperature and Thermal Diffusivity in Intact Seeds and Seeds Inside Soils by Time Domain NMR

**Maria Gabriela Aparecida Carosio**<sup>1</sup>; Luiz Alberto Colnago<sup>2</sup>; <sup>1</sup>Institute of Chemistry of São Carlos, São Carlos, Brazil; <sup>2</sup>EMBRAPA Instrumentation, São Carlos, Brazil

Soil temperature is important in agriculture and affects directly the seed germination. Some seeds may survive in high temperature environment for days, but the seedling may die in few hours. Several NMR parameters are affected by temperature and can be used to monitor it. We are showing that we can use time domain NMR to measure temperature using oilseeds as a sensor. The measurement is based on the  $T_2$  dependence of oil viscosity and temperature. Although soil type doesn't influence directly on the signal acquisition, it'll be indirectly influenced, because the seed will heat more or less depending on the soil type. This study shows it is possible to obtain information in vivo and quickly, compared with other techniques.

Poster 123

### The Chemical and Structural Characterization of Soil: A Comprehensive Multiphase NMR Approach

**Hussain Masoom**<sup>1</sup>; Denis Courtier-Murias<sup>1</sup>; Ronald Soong<sup>1</sup>; Hashim Farooq<sup>1</sup>; Werner E. Maas<sup>2</sup>; Michael Fey<sup>2</sup>; Brian Andrew<sup>2</sup>; Jochem Struppe<sup>2</sup>; Howard Hutchins<sup>2</sup>; Sridevi Krishnamurthy<sup>2</sup>; Rajeev Kumar<sup>3</sup>; Martine Monette<sup>3</sup>; Henry J. Stronks<sup>3</sup>; Alan Hume<sup>3</sup>; Andre J Simpson<sup>1</sup>; <sup>1</sup>University of Toronto, Scarborough, Canada; <sup>2</sup>Bruker Biospin, Billerica, MA; <sup>3</sup>Bruker Biospin Canada, Milton, ON

Comprehensive multiphase (CMP)-NMR is useful to investigate complex environmental samples because it has the capability to study solid, liquid, and gel-phase (HR-MAS) components without sample pre-treatment. Here we have used CMP-NMR to look at the structure and chemistry of soil colloids at the water interface in whole untreated samples. <sup>13</sup>C CP-MAS experiments on a wet and dry soil indicate that carbohydrate and aliphatic moieties are present on the surface of soils while aromatic and proteinaceous components lay buried in the solid phase and have been confirmed by <sup>1</sup>H experiments. Additionally, more penetrating solvents and multidimensional NMR were used to characterize the various soil components, strengthening the notion that soil organic matter is made of small subunits which form supra-molecular associations.

Poster 124

### Diamond Magnetometer near the Shot Noise Limit at Room Temperature

**Chang Shin**<sup>1,2</sup>; Claudia Avalos<sup>1,2</sup>; Mark Butler<sup>1,2</sup>; David Trease<sup>1,2</sup>; Scott Seltzer<sup>1,2</sup>; Daniel Kennedy<sup>1,2</sup>; J. Peter Mustonen<sup>1,2</sup>; Victor Acosta<sup>3,4</sup>; Dmitry Budker<sup>3,4</sup>; Alexander Pines<sup>1,2</sup>; Vikram Bajaj<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of California, Berkeley, CA; <sup>2</sup>Materials Science Division, LBNL, Berkeley, CA; <sup>3</sup>Department of Physics, University of California, Berkeley, CA; <sup>4</sup>Nuclear Science Division, LBNL, Berkeley, CA

The negatively charged nitrogen vacancy centers (NV<sup>-</sup>), substitutional point defects in diamond have recently been exploited in several applications including magnetometry. We operate a nitrogen vacancy (NV<sup>-</sup>) diamond magnetometer at ambient temperatures and study the dependence of its bandwidth on experimental parameters including optical and microwave excitation powers. We introduce an analytical theory that yields an explicit formula for the response of an ensemble of NV<sup>-</sup> spins to an oscillating magnetic field, such as in NMR applications. We measure a detection bandwidth of 1.6 MHz and a sensitivity of 4.6 nT/√Hz, unprecedented in a detector with this active volume and close to the photon shot noise limit of our experiment.

Poster 125

### NMR of Polyoxometallates (POM): Mo132 Meets Amino-Acids

Erhard T.K. Haupt; *Department Chemistry University Hamburg, Hamburg, Germany*

Previous studies concerning the lipophilic attraction of a ball-like polyoxometallate like Mo132 loaded with aliphatic chain internal linkers (like acetates) towards molecules with intermediate aliphatic chains like hexane, hexanol...[Chem. Eur. J. 17, 9634 (2011)] are extended to more biological interesting compounds like simple amino-acids. The surprising result is, that the amino-acids interact clearly with the Mo132-molecule, but there is no contact with the internal part of the moiety. Careful NMR-studies show (CSM and DOSY) that there is a contact, but in form of a slow exchange of the

