Dynamic Nuclear Polarization Effort

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Introduction

The EMR and NMR groups at the NHMFL are developing a new characterization tool, Dynamic Nuclear Polarization Nuclear Magnetic Resonance (DNP NMR), at high field (14.1 T / 600 MHz), to study small molecules in solution. DNP is a novel approach to NMR, providing dramatic sensitivity increases compared to traditional NMR [1], which leads to additional information about studied molecules, producing new scientific discoveries. Theoretical and experimental approaches have led to commercially available DNP systems for solid-state experiments at fields up to 19 T (800 MHz). On the other hand very little development has been made on solution DNP at high fields (greater than 1 T). Our group is leading the technological development in this area.

Concept

High-power 395 GHz microwaves are used to polarize electron spins (via EPR excitation) associated with radicals introduced to the solution. The electron spins in turn polarize hydrogen nuclear spins in the molecules of interest via the Overhauser effect. This method increases the number of polarized nuclear spins tremendously, thereby resulting in very high NMR sensitivity. In order to build a robust high field solution DNP system in an efficient manner our team has acquired standard components from commercial vendors. The remaining components are being designed in collaboration with Thomas Keating Ltd in the UK, or they are being designed and manufactured in-house.

Instrument development

Fig. 1 shows a schematic of the solution DNP NMR system. The magnet has been installed and energized. The console will be installed in January 2014 allowing for preliminary testing of the sample cavity and holder. The microwave quasi-optics, which control the beam power and polarization, and the probe, are in their final design stage. They will be installed in March 2014. The gyrotron, completing the system, will be installed in April 2014.

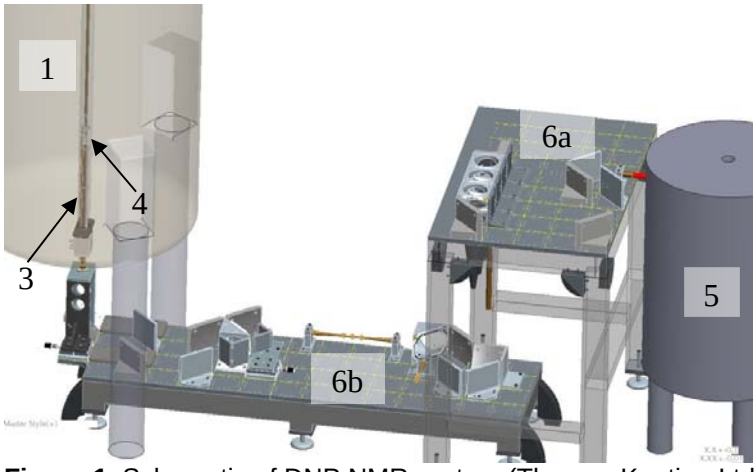

Figure 1. Schematic of DNP NMR system (Thomas Keating Ltd.)

1) Magnet
commercial - Oxford 600 MHz
2) Console (not shown)
commercial - Varian INOVA
3) Probe
in-house modified Varian
4) Sample cavity and holder
in-house design and manufacturing
5) Gyrotron, microwave source
commercial - Bruker 395 GHz
6) Microwave quasi-optics
collaboration with Thomas Keating Ltd
a - power control
b - polarization control

Conclusions

The high field solution DNP NMR system is in its final development stage. It will be operational in 2014.

Acknowledgements

We acknowledge the National Science Foundation (MRI grant # CHE 1229170) and the State of Florida (for matching funds) for financial support.

References

[1] Griffin, R., *et al.*, Phys. Chem. Chem. Phys., **12**, 5737–5740 (2010).