NMR @ Sussex

University of Sussex

Iain J. Day

i.j.day@sussex.ac.uk

Department of Chemistry and Biochemistry

University of Sussex, Falmer, Brighton, BN1 9QJ, UK

Equipment and Facilties - solution state NMR

We are fortunate to be equipped with three state-of-the-art solution state NMR spectrometers:

Varian VNMRS 400 MHz
9.4 T / 54 mm Premium Shield Magnet
^{1}H-^{19}F/^{31}P-^{15}N AutoX DB Probe

Varian VNMRS 500 MHz
11.75 T / 54 mm Premium Shield Magnet
^{1}H{^{31}P-^{15}N} AutoX ID Probe
SMS-50 Autosampler

Varian VNMRS 600 MHz
14.1 T / 54 mm Premium Shield Magnet
^{1}H-^{19}F/^{31}P-^{15}N AutoX DB Probe
^{1}H{^{31}P/^{13}C/^{15}N/^{2}H} AutoPenta Probe
9 Sample Carousel

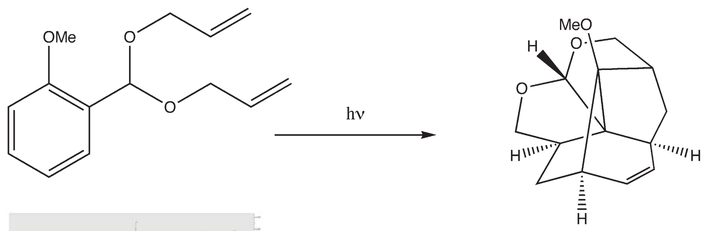
Solid state NMR

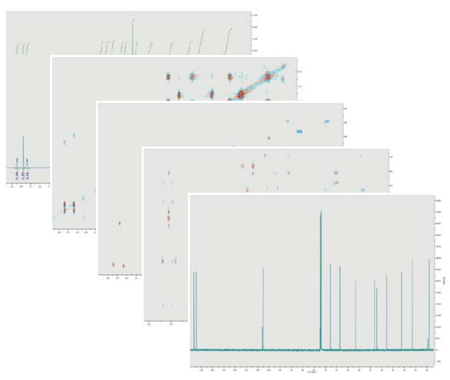
We are also equipped with solid-state NMR capabilties.

Bruker Avance DMX 400 MHz
9.4 T / 89 mm Spectrospin Magnet
4mm ^{31}P-^{15}N{^{1}H} MAS Probe
^{1}H gHR-MAS Probe
10 mm ^{31}P-^{109}Ag{^{1}H} solution probe

Structure Elucidation

In collaboration with Dr Clive Penkett we have worked on determining the structures and stereochemistries of products from various photo-cycloaddition reactions. These reactions provide quick and efficient routes to molecules with a high degree of structural complexity.





^{1}H and ^{13}C

COSY and TOCSY

gHSQC

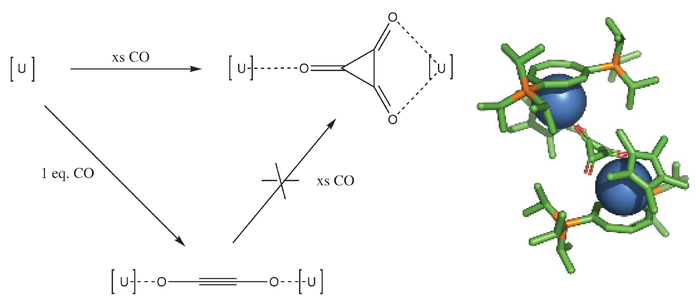
gHMBC

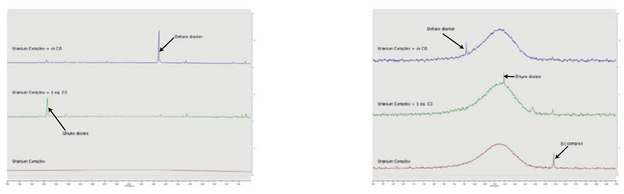
gH2BC

NOESY and ROESY

Organometallics

Work in Prof. Geoff Cloke's group is concerned with reactions of uranium complexes with CO. We have employed ^{13}C and ^{29}Si NMR with a view to understanding the mechanism and intermediates of these intriguing reactions.





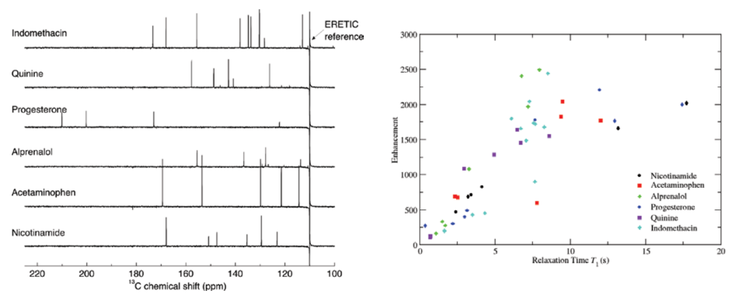
Multinuclear NMR studies with other groups in the department have involved a wide variety of nuclides including ^{119}Sn, ^{199}Hg and ^{207}Pb amongst others.

NMR Research

Our NMR research interests are based around two areas: (i) sensitivity enhancement and (ii) reaction kinetics and time resolved NMR spectroscopy.

Sensitivity Enhancement

Recent work in this area has focused on applications of dynamic nuclear polarisation (DNP) for small molecule NMR.



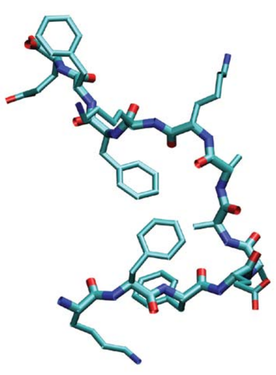
Time-resolved and kinetic NMR

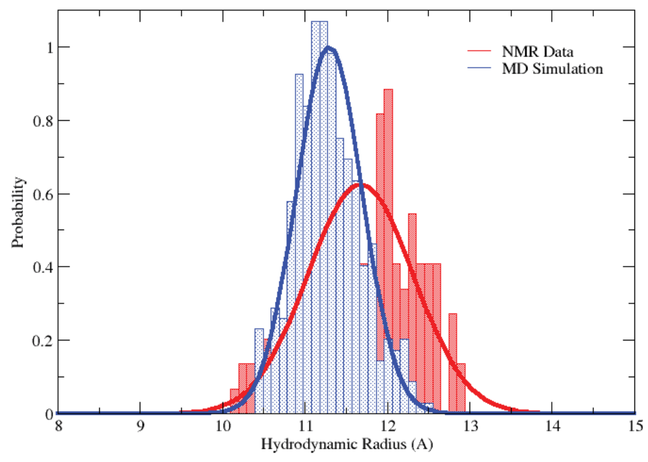
In collaboration with Prof. P. J. Hore (University of Oxford) and Dr K. Hun Mok (Trinity College Dublin) we have developed methods for stopped-flow NMR and demonstrated its utility for the study of protein folding and real-time NMR spectroscopy.

Protein and Peptide NMR

In a joint project with Drs Louise Serpell and Peter Varnai we are interested in the formation of amyloid fibrils and are undertaking combined NMR, biophysical and computational studies.

One example of this is work measuring hydrodynamic radii in solution and comparing results with molecular dynamics simulations. We have employed the PG-SLED variant of the DOSY methodology and have obtained good agreement between experiment and theory.





Services Available

We are pleased to be able to offer external users access to our facilities. We offer a full range of services including:

- Routing data collection (including heteronuclear and VT experiments),
- Advice regarding appropriate choice of experiments,
- Complete data analysis, with the option of a written report.

We are also interested in fully collaborative projects. Additionally, the department is equipped with an excellent mass spectrometry suite and X-ray diffraction facilities which would be available to support any NMR projects.

Competitive access rates for external academic and industrial users are available on request.

Contact Details

For further information about NMR @ Sussex, or to discuss if we could assist you in your research, please contact:

Dr Iain J. Day
Department of Chemistry and Biochemistry
University of Sussex, Brighton, BN1 9QJ, UK

T: +44 (1273) 876622
F: +44 (1273) 876687

http://www.sussex.ac.uk/Users/ijd22/nmr_service/

E: i.j.day@sussex.ac.uk