UNIVERSITY OF LIMERICK
OLLSCOIL LUIMNIGH

Bernal Institute

Solid-State Nuclear Magnetic Resonance Spectroscopy NMR

Overview

- Our solid-state NMR facility is located in the Bernal Institute and houses a Bruker Avance III HD wide-bore 9.4 T ($\nu_0(^1H)$ = 400 MHz) NMR spectrometer capable of three-channel operation.
- The facility is accessible to Bernal staff and students, as well as academic and industrial collaborators in Ireland and internationally.

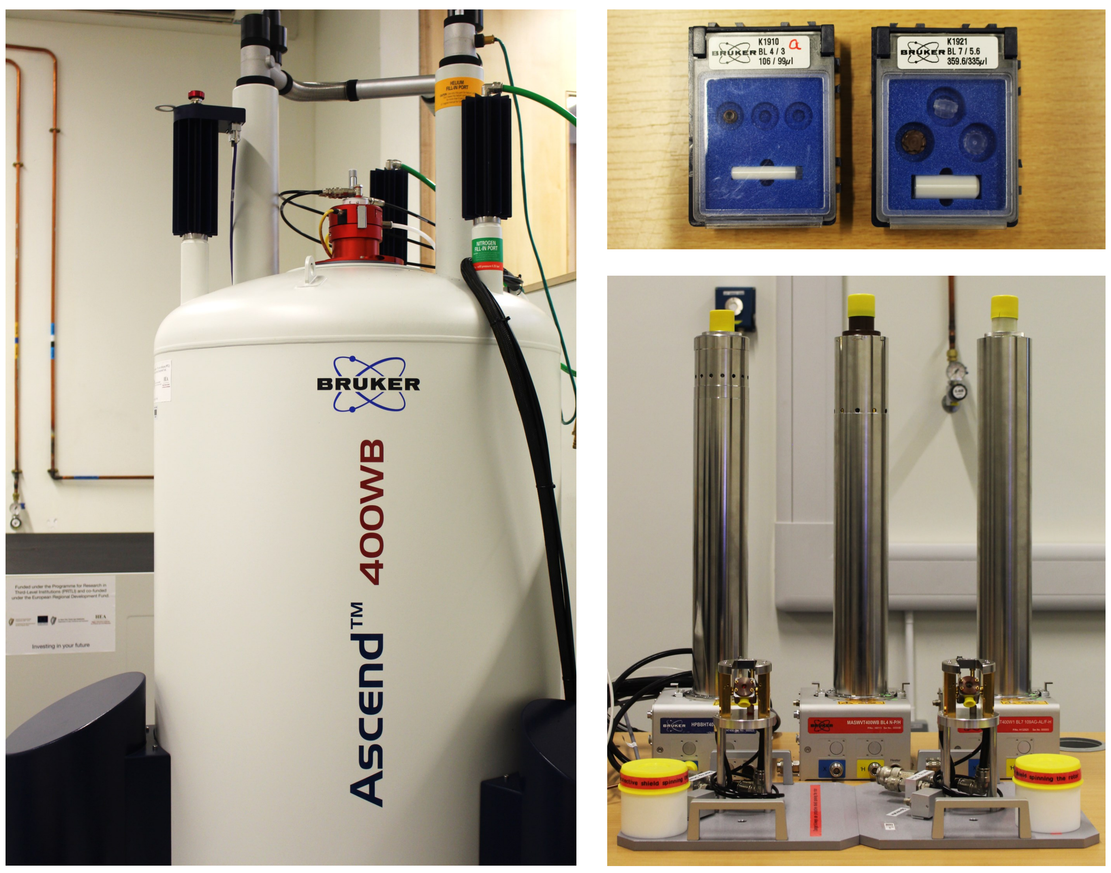

Figure 1. 9.4 T solid-state NMR magnet, probes, rotor spinning test stations, and sample rotors.

NMR Capabilities

- Capable of producing solution-like NMR spectra of solid materials via magic angle spinning (MAS) with MAS frequencies up to 15 kHz.
- Several MAS probes available, including 4 mm double resonance (H/X), triple resonance (H/X/Y), and 7 mm double resonance (H/X) probes with a collective frequency range from ^{109}Ag to ^{31}P and from ^{19}F to ^{1}H.
- Variable temperature operation from approx. −40 to +300 °C. Sub-ambient temperatures achieved *via* a BCU II pre-chiller unit operating with a dry air supply.
- 5 mm single-channel (X) stationary probe with a frequency range from ^{109}Ag to ^{31}P and variable temperature capabilities up to +150 °C.
- 4 mm and 7 mm rotor spinning test stations available.

Research Applications

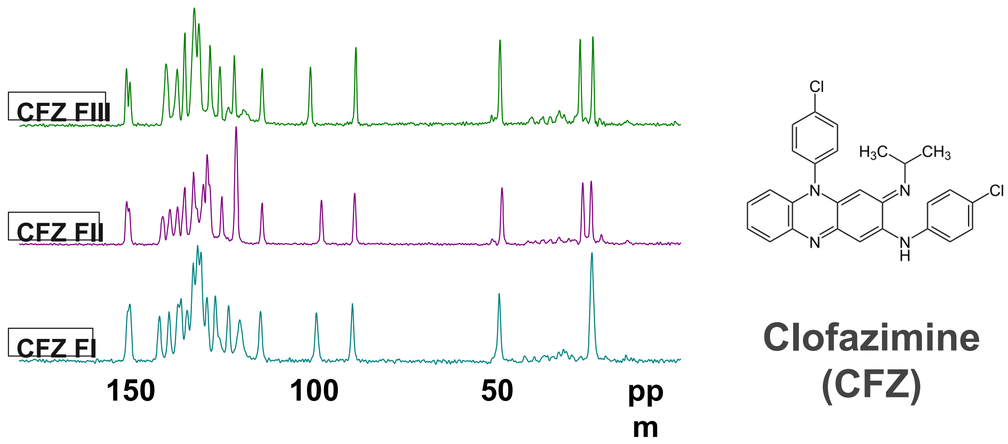

Figure 2. ^{13}C NMR spectra of solid forms I, II, and III of clofazimine acquired at a magnetic field strength of 9.4 T using the cross-polarization pulse sequence.

- Many academic and commercial applications in areas such as pharmaceuticals, biomaterials, modern materials, and energy and environment.
- NMR spectroscopy is used to determine and/or refine the molecular structure and dynamics of both crystalline and amorphous materials, as well as nanomaterials.
- Routinely used to distinguish between solid forms of materials, e.g., solvates, polymorphs.
- Able to characterize materials in the presence of others, e.g., active pharmaceutical ingredients in excipients, as well as characterize molecule-matrix and guest-framework interactions.

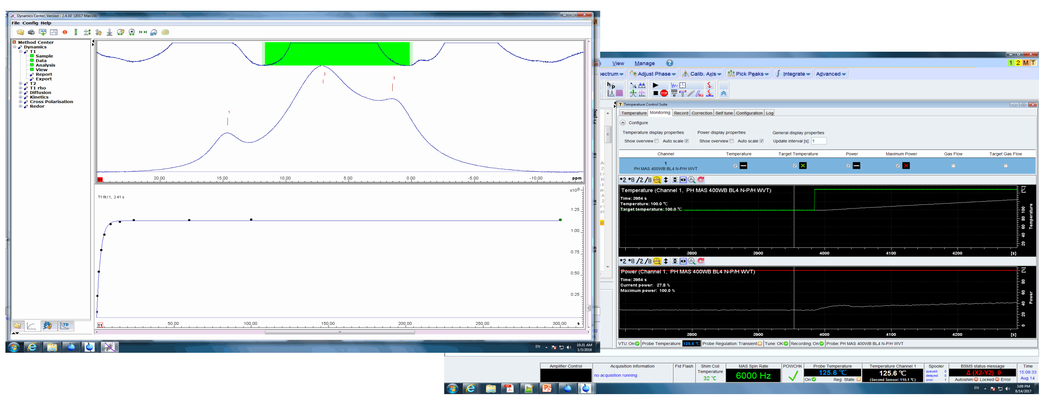

Figure 3. Bruker TopSpin software displaying ^{1}H T_1 relaxation data and variable temperature experiment monitoring.

Potential Collaborations

- Contract engagement
- Project based
- Innovation partnerships
- IRC Enterprise partnership scheme (PhD & PDF)
- Training seminars/workshops
- Graduate and undergraduate training

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