What is the collective noun for solid-state nuclear magnetic resonance spectrometers?

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A few weeks ago saw the University of Warwick in the UK Midlands host a very successful two-day conference for the AkzoNobel analytical science community with attendees from the UK and Europe. It is not my intention to advertise any particular location for running conferences or to present anything of the content of the meeting, but as part of the event we enjoyed interacting with some of the staff of the superb facilities the University has available to support non-Warwick-based researchers to use supporting Open Innovatione.

Background

Amongst some excellent science seen on our tour, the solid-state nuclear magnetic resonance spectroscopy (NMR) facilities at Warwick stood out; not only due to the large number of magnets, eleven (maybe the collective noun could be "Kettle" as used for many hawks?), but also the attitude and approach of the staff.[1]

Interestingly, the solid-state NMR facility is located within the Physics Department. This was described as essential due to the complexity of the mathematics involved (seems like a challenge, chemists!). These facilities are in addition to the strong NMR Spectroscopy presence in the Chemistry Department with four open access 300 MHz and 400 MHz instruments and four high-field instruments at 500 MHz, 600 MHz and 700 MHz.

Why is solid-state NMR so different?

For those who do not practise solid-state NMR, it is worth reviewing why this field is so different from its liquid-state cousin. The easy answer is "it isn't". The interaction between the nuclei of the atoms in the sample and the magnetic fields applied by the spectrometer and the superconducting magnet are the same. However, what makes solid-state NMR a field worthy of placing in a different faculty is time and anisotropy.

Within an NMR spectrometer, the electromagnetic field is strongly directional. It interacts with the rotating nuclear spins as long as there are isotopes which contain an odd number of protons and/or neutrons, which give an intrinsic magnetic moment and angular momentum to the nuclei. As the applied field is directional and the magnetic moment of the nuclei is also directional, you would expect to have different interactions depending on whether the fields align or not; similar to a polarisation experiment in optical spectroscopy. This is where time comes in. In a standard solution-state NMR experiment, the sample molecules are rapidly moving around compared to the time scale of the experiment. This averages out the anisotropic interactions so you normally get nice narrow signals to interpret. In solid samples the motion is no longer present, so the different orientations of the molecules in the solid sample to the applied field cause a large broadening of the observed signal.

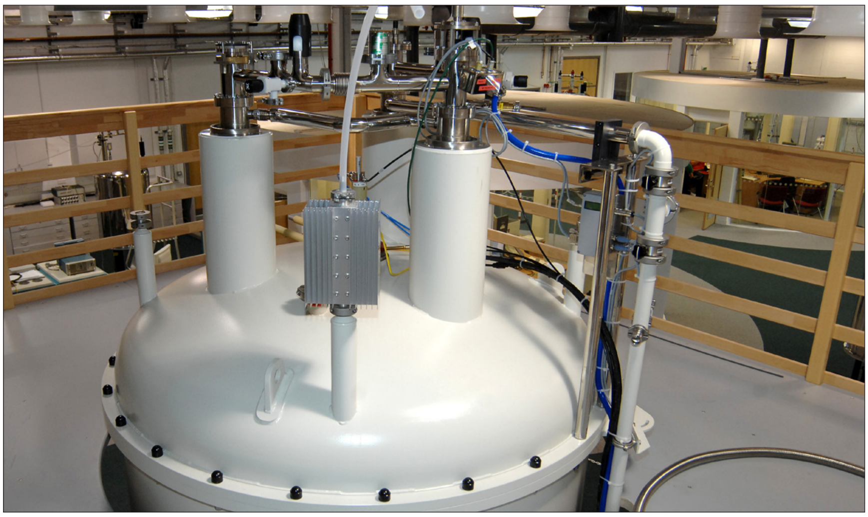

Figure 1. The UK's National Facility's 850 MHz wide-bore magnet hosted at Warwick.

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This is not to say that this broadening necessarily has to be avoided, as it is carrying interesting structural orientation information about the sample being analysed. If you are looking for liquid-NMR-like narrow peaks for your sample interpretation, there is a simple experimental way to eliminate the broadening by imitating the averaging motion in solution-state NMR: rapidly rotate the sample. This so-called magic angle spinning succeeds in averaging out some of the broadening, but is only partially successful. However, in the age of the Internet, this column cannot be allowed to descend into a beginner's guide to solid-state NMR, so let us move on to why solid-state NMR is such an important facility to have maintained as a state-of-the-art Open Innovation resource.

Applications

As suggested above, the root causes of the broadening which are lost in conventional solution-state NMR can be useful in solid-state NMR, providing structural information on the solid being measured. The higher field strengths give access to a wider variety of more complex experiments probing macromolecular and domain information often unavailable by other techniques. These include interactions between nuclei across space rather than through bonds, crystal domains and defects, hydrogen bonding, and supramolecular structures. Although biological applications are often headline-grabbing, many industrial materials science questions are capable of being addressed through solid-state NMR.

Clearly, the complexity of the systems, and especially the dynamic biological systems, require advanced computing and modelling capabilities as well as the necessary hardware. All this investment would be wasted if a vastly more important foundation were absent. The most precious resource of all is the scientific staff capable of operating the technical side whilst displaying the people skills to successfully communicate and interpret the needs of their varying customer base. I found it interesting that one of the duties of the facility manager—alongside all the technical responsibilities you would expect in such a role—was "Promoting a positive and welcoming feel to the Facility". This has often been overlooked when staffing and operating national-scale facilities in the past. The successful long-term use of such facilities often relies on the building of strong open relationships between the staff and their customers whether in industry or "rival" academic institutions.

With EU-originating funding playing a key role in the establishment and ongoing world-class delivery of this facility, it is sobering to read the eloquent submission to the House of Commons Science and Technology Committee in August on the potential effects of the Brexit vote.[2]

Computing

The results of the various experiments are usually processed using the vendor software. However, for a facility aligned with the Open Innovation agenda I was interested in how the data is distributed and made available to their customer base. Non-critical data is served to the user community through a dedicated data archive server off-spectrometer. Those wishing to process the data themselves can do so by downloading their data to their local IT environments and work using the standard vendor software at their own locations. Many research institutions do not have their own NMR data processing capabilities and, where this is the case, the facility will assist in providing access to the necessary software.

For industrial partners or those with heightened secrecy requirements on IP or other grounds, their own data dissemination routes are set up to meet their specific needs as necessary.

Conclusions

Six years have passed since the UK 850 MHz Solid-State NMR Facility was original opened and they are currently halfway through their current 3+2-year funding period (Figure 3).

The facility has quite a complex management and oversight structure, which is very transparent in its operations. Their 2015 report, for example, publishes their Customer Satisfaction Survey which, as someone tied up in evaluating such exercises over recent years, reads very well.[3] I think the future of this facility post-Brexit with the timing of their subsequent funding rounds and broad international scientist population may well serve as a potential bell-weather for a post-Brexit UK science landscape. They need to be able to keep up with, for example, the investment available to their colleagues in a country with a much lower GDP such as the Netherlands highlighted in 2013.[4] It would be a tragedy if they end up scratching around for cash to keep the facility open rather than concentrating on delivering world-class science like our colleagues in the uncertain world of Canadian High Field NMR facilities.

So, going back to the original conundrum at the top of the article, maybe we should be looking at proposing "Wisdom" as the collective noun (after a Wisdom of Wombats—for those who love the added alliteration!). Hopefully, wisdom will also shape UK government funding policy in a post-Brexit world and they will deliver on their promises that overall funding for such facilities will not suffer and we will not see the smile wiped off Steven's face.

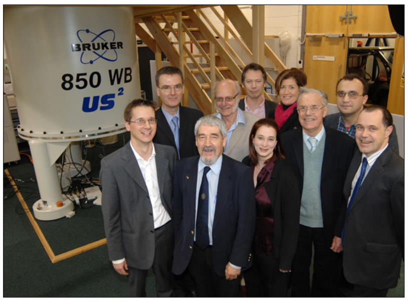

Figure 2. UK NMR nobility turnout for the original symposium celebrating the opening of the UK facility in 2010. Steven Brown is the scientist smiling happily on the very left of this group, to his left is the then chief executive of EPSRC, who are the principal funding agency (with partial support from BBSRC), with others compromising the then National Management Committee.

References

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