Understanding the Current Portfolio and Resourcing Implications of NMR Infrastructure Underpinning World Class Physical Sciences

1. Context

There is an undoubted link between the availability of modern state of the art infrastructure and the ability to produce world-leading research. To maintain the UK's position as one of the world leaders in research, understanding the implications of the more capital constrained world of 2012 and beyond for the future availability of high class research infrastructure is critical. The situation with regards to research equipment is complex as the advances in techniques and technology have meant that the ability to achieve particular levels of performance (e.g. given signal-to-noise, resolution, etc.) has become relatively much cheaper, but at the same time the increasing sophistication of the state of the art drives the costs up of providing leading-edge facilities. NMR is a very widely used experimental technique within the physical sciences and can be used as an exemplar technique to understand the challenges of technique provision to scientists and the community. This document summarises some of the key points that arose from a consultation in November 2012 with the 25 heaviest higher education institution (HEI) users of NMR infrastructure in the physical sciences community. Whilst undertaking this consultation a small complication arose in that with the availability, at short notice, of some capital funding for chemistry infrastructure a call was issued to Chemistry Departments in the final quarter of 2012. The remit of the call (Core Capability for Chemistry Research) overlapped to some extent with the information requested here. However this has turned out to be an advantage as Chemistry Departments are the heaviest users of NMR and they had to develop a more detailed scientific case for NMR equipment replacement. Hence this report has drawn on two sources of information – (i) that supplied directly in response to the consultation request from EPSRC, and (ii) the information about NMR within the call for Core Capability for Chemistry Research.

It was clear from all submissions that NMR certainly continues to be an absolutely indispensable key underpinning technology across almost all areas of physical science with areas identified including civil engineering, chemical engineering, physics, chemical biology and materials science. However the dominant user of NMR is the Chemistry community where NMR facilities are regarded as essential to provide an internationally competitive chemistry environment. This observation is backed up by bids to the Core Capability for Chemistry Research call where the 20 bids from 22 universities requested for NMR in the immediate future £8.2M (part A) and near future £19M (part B), making up a sizeable fraction of the total requested under this call. Under part A approximately 40% of the approved funding went to NMR instrumentation. This in itself shows the back log of outdated infrastructure that has built up and emphasises that the sector (which is taken here as a combination of HEIs, the research and funding councils and indirectly Government) is some way from understanding how to make such research infrastructure sustainable, and therefore being able to suggest actions to deliver sustainability, although it also became clear progress has been made. The survey has provided some additional insight as to the state of operation of this current NMR infrastructure and the requirements for immediate (< 2 year) upgrade, as well as the anticipated needs of the physical sciences community in terms of leading-edge developments in the relatively near term (2-5 years).

The 2010 Wakeham Review on full economic costing (fEC)[1] provides some key context for understanding the sustainability of equipment infrastructure. In addition this survey takes place against the background of significant reductions in capital streams for such research equipment in the current Comprehensive Spending Review period 2011-15. The RCUK response in the context of both of these is captured in to their report 'Efficiency 2011-15: Ensuring Excellence with Impact'. A key consideration from that report was the effective and efficient utilisation of existing and new assets across the research base. This survey provides some real insight into this agenda as well.

2. Observations on Institutional Behaviour and Operation with regards to NMR Infrastructure

The information supplied revealed that institutions and researchers involved in the physical sciences in the UK exhibit some interesting and genuinely new modes of operation and behaviours with respect to NMR infrastructure. NMR used as a core underpinning technology is often concentrated in a facility run by a Department (usually Chemistry) or Faculty. Although some universities have succeeded in bringing all such NMR equipment whether used by the Physical Sciences or Life Sciences into a single facility, the norm for large research intensive HEIs to have one facility associated with each area. Such a decision is often based on the spatial separation of these disciplines within the HEIs and that the optimisation and configuration of the facility often has to be quite different in these two disciplinary cases. There are examples of HEIs where there are integrated offerings of departmental/faculty facilities together with specialised equipment of a research group in the one location, and others (more common) where the facility and research group instrumentation are separately located. It should also be noted that some universities have not yet managed to concentrate underpinning service equipment even within a single physical location, but this is the exception. This survey shows that centralisation of facilities can often be achieved providing that there is a will within senior management of a department/faculty/university for this to occur and can bring several benefits and may be necessary in order to realise some of the additional possible benefits suggested below.

An area where national policy is clearly having a major impact and change of behaviour is the efficiency and equipment sharing agenda. One immediate benefit is that there has been a really significant drive resulting from this agenda in developing and populating databases of the capital infrastructure within universities. Hence many contributions indicated that providing the information requested for this survey was, for the most part, very straightforward, but also indicated that until very recently it would have been far from so. EPSRC funding via Impact acceleration accounts was cited as one of the impetuses to this. Many of these databases are already searchable publically. An example of this is the one at Leeds where a detailed taxonomy has been developed for classifying equipment in their database which is readily searchable.[2] This change has had several benefits in that HEIs could better understand the scale of the financial liability associated with infrastructure renewal to be addressed and could now also better allow coordinated development of procurement strategy and equipment sharing with partners to be contemplated. It was pleasing to see that most universities had come to grips with the need to back up such facilities with skilled personnel, with the common model being that an academic member of staff has leadership responsibility, backed up at a relatively high level with an experimental officer plus some technical back-up. Although it is expected that these support

[1] 2010, Financial Sustainability and Efficiency in Full Economic Costing of Research in UK Higher Education Institutions.

[2] The Leeds University equipment database can be found at https://esms.leeds.ac.uk/default.aspx - typing NMR into this page reveals the NMR equipment available.

personnel costs will be significantly recovered from funded research, most universities have underwritten these positions with indefinite contracts.

3. Current Capability and State of NMR Infrastructure for UK Physical Sciences

The survey indicated some interesting characteristics, with in the universities surveyed the portfolio of instruments primarily used for research[3] split 133 for solution NMR work and 28 for solids[4]. The NMR infrastructure within the physical sciences is clearly concentrated within Chemistry departments who regard the provision of high quality NMR facilities as absolutely essential. Hence much of the NMR equipment out there is regarded as what should be present in the well founded laboratory. Here the researcher would use NMR either in automated mode or via a walk-up/technician operated facility as a service rather than a piece of core research integral to the research objects of the project. It should be noted that the other area where NMR is also used in this way as a facility is within the Life Sciences where NMR is primarily regarded as a technique for protein structure determination, although this and related structure determination is becoming increasingly important for aspects of cutting-edge synthetic chemistry. This survey has tried to disentangle equipment on the basis of the primary funding source for the equipment or for the research carried out on that equipment (i.e. BBSRC, Wellcome is not included), although inevitably there is some degree of arbitrariness to this split. The second mode of use of the equipment is when the technique or its application is the primary object of the research of a researcher or group of researchers. The UK has a first class reputation in leading the development and application of NMR techniques and there are groups scattered across all physical science disciplines using NMR in this way.

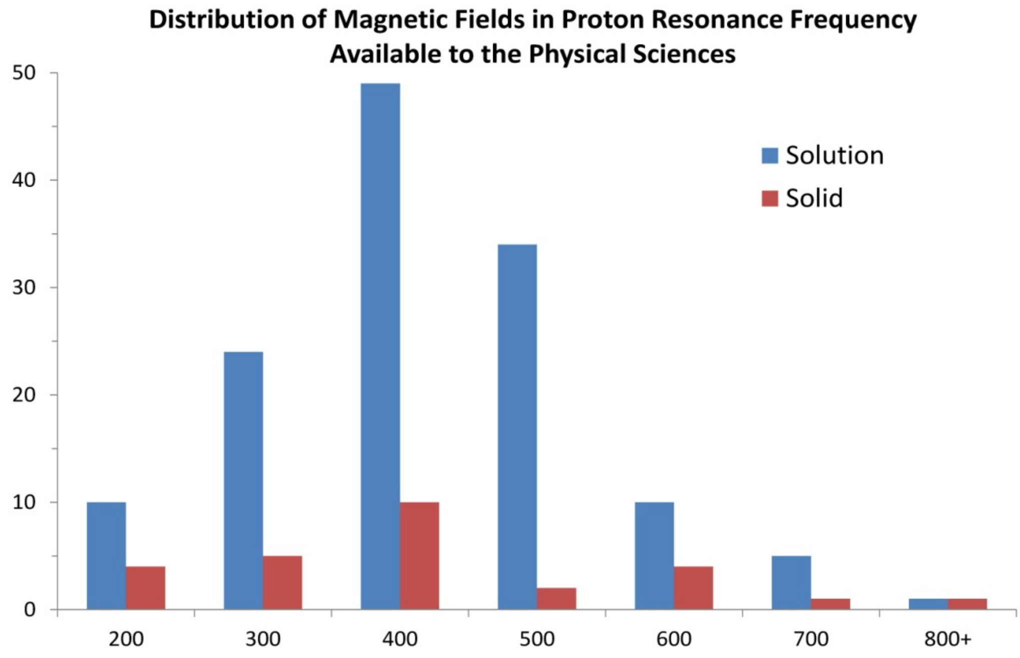


Figure 1. The spread of strengths NMR spectrometers available to the physical sciences above 200 MHz proton frequency.

[3] Equipment primarily assigned to undergraduate teaching has not been included
[4] The split is on the basis of the whether or not the equipment was primarily specified for solids and does not include the provision of solid accessories on solution instruments nor systems below 100 MHz proton operation.

The spread of equipment (Fig. 1) revealed by the survey was intriguing. The dominant field for both solution and solid state NMR work was 9.4 T (400 MHz proton). Given how long higher magnetic fields than this have now been routinely available it is a little surprising that this field remains the most used.

The four main observations on the equipment data are:

(i) The number of instruments supporting solution NMR in the range 200-300 MHz comprised over 25% of the current portfolio. This is probably a result of the development of the portfolio by accretion rather than active replacement, which is perhaps a natural tendency, particularly when one of the key pressures is capacity issues. However this approach then stores up a problems in terms of capital replacement;

(ii) Only 13% of the portfolio for solution NMR is at 600 MHz and above, with only one instrument at 800 MHz[5] where physical sciences activity has clear access;

(iii) Although the proportion of instruments at 600 MHz and above is higher in the solid state NMR community at 21% there are only two instruments for solids work above 600 MHz (i.e. one 700 MHz and the national 850 MHz facility);

(iv) Cryoprobes brought significant gains in sensitivity in solution NMR, but the number of solution instruments with associated cryoprobes was much lower than expected given how long this technology has now been around.

The survey also captured some age information. More aged equipment becomes physically worn out requiring more repairs and is of lower inherent sensitivity. However what becomes more of a limitation in enabling internationally competitive research is the range and sophistication of experiments that can be performed on older instruments. So NMR technology improvements over recent years include more routine access to gradient shimming, shaped/adiabatic pulses, multi-channel operation and wider range routine X-nucleus detection, with much of this under automation, fast magic angle spinning (MAS) and cryoprobe experiments. A concrete example where previous generation consoles are severely limiting the complexity of experiments that can be undertaken is with pulse-shaping. The turnover time for such technology is probably around 7 years for console and probes, when it then becomes 'last' generation. Ten years is probably the best guide for a combination of when such equipment becomes really last generation and the actual physically reliable longevity of the equipment. The age profile of the consoles (Fig. 2) shows around 40% could be regarded as roughly current generation, which is a positive number. On the down side approaching 50% of the portfolio is 11 or more years old which in an ideal world should be replaced and is therefore a big capital liability for the sector.

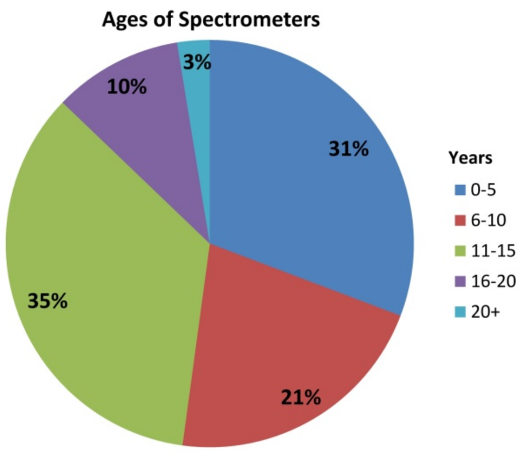


Figure 2. The age profile of NMR spectrometer consoles being used within the physical sciences.

There is then a double loss of efficiency with older 'last' generation equipment in that adequate, but less informative experiments are performed. Cases were cited where keeping instruments running using a 'patch and mend' approach, sinking quite a

[5] Only one 800 MHz instrument was clearly located in an environment where significant physical sciences work was being undertaken but it is likely that much of the work even on that instrument was life sciences funded.

bit of support time costs into them. Overall usage figures for most instruments were commendably high (> 80% on a 24/7 basis). Many systems had had upgrades with robotic sample changers and for solution work the sensitivity advantages of implementing higher fields and cryoprobes was certainly evident, but nowhere near as widespread as expected to give the sensitivity advantages. It should be emphasised that improved sensitivity has two advantages namely the improved throughput and hence efficiency of operation *and* the range of experiments/samples that can be contemplated increases.

This then brings one to consideration of availability of magnetic fields which also plays into the sensitivity arguments as magnetic field is a fundamental driver of sensitivity, but also bringing the added advantages of greater resolution. In solution state experiments, such as shift-resolved 2D methods the resolving ability of the experiments (e.g. TOCSY, HSQC) improves as the square of the applied magnetic field. The advantages of this resolution are seen in better resolution of compounds in complex mixtures (e.g. metabolomics) and in detecting very small differences in structure. With the increased sensitivity many more sensitivity limited experiments become possible, such as detection of very dilute components in mixtures and low level reaction intermediates. For solids there are also a big advantages of higher magnetic fields through increased sensitivity, but especially for the observation of quadrupolar nuclei where again resolution improves rapidly with increasing magnetic field. There has been a gradual shift to higher fields, but lower fields have been retained for too long. As an out and out research tool lower field solution instruments, certainly below 300 MHz should be replaced. Even if a 300 MHz system were adequate, the greater sensitivity and throughput means that the underpinning university facility specific solution NMR equipment should be 400 and 500, with significant cryoprobe availability at 500 MHz and above. There should be increasing availability of 600 MHz within such facilities. It was noted in several submissions that access to 500-600 MHz solution state NMR is now essential for competitive research within Chemistry Departments, as lack of on-site access can significantly impact on productivity and potential for work-leading status of such research.

Solid state NMR has until relatively recently been regarded as a specialist technique, but several cases were made for chemistry communities, such as those with large materials chemistry research efforts, as now needing to directly associate solid state NMR capability with their departmental/faculty facilities. It should be noted here that because of the higher cost of wide bore (as opposed to standard bore) magnets and the factors determining line widths it is the case that slightly lower field 300-400 MHz should apply as standard work horse instruments for solids experiments than for solution work.

As highlighted above the survey revealed that for the question of really leading-edge high field equipment, there are several potentially serious weaknesses in the UK provision supporting physical sciences. For solution NMR there are surprisingly few instruments at ≥ 700 MHz available to the physical sciences community (although there is availability for the Life Sciences where the field is essential for the larger protein molecules) and similarly for the solid state community above 600 MHz there is only one group based instrument and the national 850 MHz facility. That this is a problem can be seen by comparison with the main European competitors (e.g. France, the Netherlands, Germany) where there has been systematic development of networks of instruments at 700 MHz and above for both solution and solid state NMR. An interesting observation was made with regards to a number of European calls for supporting high level infrastructure that in exchange for European access for part of the time on such instruments, significant recurrent funding (in particular helping with the funding of the support posts) can be earned. However to be attractive to be parts of such networks the equipment needs to be leading-edge, which for NMR is often directly related to the magnetic field. At the moment the UK is often not really competitive enough to be a part of these potentially lucrative and prestigious networks.

At the extreme in the discussion over the provision of leading-edge spectrometers is the availability of ultrahigh magnetic field, which impacts on the physical sciences. However the scale of the necessary investment (> £16M) should feed into a discussion which is probably cross-council. In the near to medium term (up to 2020) the UK needs to contemplate its provision of ultrahigh field NMR (> 1 GHz). Orders for such ultrahigh field instruments have been or will shortly be placed from Germany, Italy, Switzerland and the Netherlands. The Netherlands have included ultrahigh field NMR as a priority of their large facilities roadmap released in May 2012, where funding of 18.5 MEuro for the first 1.2 GHz instrument was announced that is intended to be part of an eventual extensive network of very high field instruments of which several are intended to be above 1 GHz. All of this evidence is pointing towards a similar hierarchy of NMR infrastructure that maps onto the classification of high performance computing into tiers 1-3. A similar classification may be helpful here and with other experimental techniques.

A question was also raised as to being clear where other real strategic needs reside for NMR. For example there is a definite requirement in the physical sciences community for provision of specialised facilities for extreme diffusion measurements, novel implementation within various engineering applications, wider temperature capability, along with relevant imaging capability. In the drive for ever higher sensitivity in NMR cold or 'cryo'probes were a key step forward through the gain of a factor up to ~ 4 in signal and hence more than 15 in signal-to-noise. This has become even more useful as X-channel cryoprobes have become available. The recent renaissance in dynamic nuclear polarisation (DNP) offers possibilities for signal enhancements of ~10-330. RCUK funding for fundamental developments in DNP has allowed the UK to remain competitive on the development front. However recently commercial instrumentation at 9.4 and 14.1 T has become available that allow the user community to begin to evaluate the real worth and likely impact of such DNP technology. Some countries have responded rapidly, with for example a DFG call in 2011 announcing funding in October 2011 of three DNP spectrometers across the science base including the physical sciences. In the UK having no new generation commercial DNP instrumentation to act as a national facility and focus for understanding the range of impact of this technique is a weakness. Developing such a facility should be a strategic priority.

4. Sustainability

4.1 Financial

The data collected indicated that a patchwork of funding had been used in the past to fund the NMR infrastructure within physical sciences which is most likely repeated with other instrumentation for other techniques (e.g. mass spectrometry, electron microscopy) and disciplinary areas (e.g. Life Sciences). In this survey the sources of funding of the original equipment quoted included Multi-project Equipment, JIF, JREI, SRIF, CIF, Regional Development Agencies, Universities' own funds, responsive mode grants and donations. As equipment or capital calls came along there was often a response that filled a short term need with a tendency to meet demand by an expansion of capacity rather than upgrading and/or replacement. It is largely unclear if analysis was undertaken as to the funding replacement strategy and the sustainability of the infrastructure prior to purchase i.e. could the capital funds for replacement be generated within the business plan for the equipment/department/university. Many of these funding schemes were pre-fEC so it is to some extent legitimate not to have factored in the cost of replacement as it was expected future Government capital funding lines would emerge to cover this. However we should be in a very different position with fEC meaning that sustainability should be built into the costs. With the move to fEC funding from RCUK has always only been at the 80% level under dual support, but has got tighter as Wakeham efficiencies have been sought. Under the transparent approach to costing (TRAC) HEIs in the TRAC calculation of the costs include equipment at the insured replacement value irrespective of the financial accounting position on the depreciation.

If equipment is to be used as a specialist facility and charged across a broad portfolio of activities it can be designated as either a Major (MRF) or Small Research Facility (SRF). In the original fEC guidance on these was to suggest a divide where the replacement cost or annual cost was < £300k. The main difference in the calculations of rates was that SRFs are only really based on the direct costs (it seems that other directly associated costs e.g. technical are a little grey) whereas MRFs could include all costs, especially the inclusion of depreciation. The number of NMR facilities that are charged as MRFs is very small, although quite a few more are charged as SRFs. It would appear that almost no piece of equipment, but perhaps more importantly equipment used as a facility, is yet fully self-sustaining. This does *not* appear to be a problem with the actual utilisation rate, which is the number at which the charging rate is based on, but rather the mix of activities which subsequently mean it is not possible to fully recover costs. That this is a real problem now has been brought into sharp focus with the significant reduction in capital streams most notably that available to Research Councils for grants and the Funding Councils (e.g. for CIF). The survey indicated for many of the instruments that need upgrading in the near to medium were expecting very significant funding from EPSRC. Given the current and projected level of capital available funding across all equipment available to the EPSRC there is probably a significant mis-match between supply and demand of such funding. Many 'workhorse' solution NMR facilities within Chemistry Departments are run as SRFs. Yet there is a compelling case from the evidence here that even run under fEC this is not a sustainable situation and it is would be timely for EPSRC (along with the other Research Councils) to fully understand the operation of this fEC model and how it needs to be modified to achieve sustainability. Wrapped up in this sustainability question is the use of such infrastructure by PhD students. With students no longer eligible to be funded from projects, the funding sources are mainly from Doctoral Training Accounts or Centres for Doctoral Training the universities only get the fees plus the RDP element of QR-funding totalling around £7,000. Such funding is well below that necessary to make it genuinely financially sustainable and needs to be corrected so that there is not a tension between allowing our PhD students access to really leading-edge equipment so that they can be trained to world-leading standard and the sustainability of the equipment.

In the submissions several points were made about various aspects of funding and that greater clarity over what the different funding streams are meant to fund so that there is greater transparency over the income streams and the way they are intended to be mixed together to meet the costs of research. Hence a key point made was clarity over the responsibility for funding different elements of the spectrometer portfolio and once this clarity was achieved what medium term certainty was possible over the funding streams to allow planning. It is also clear that much of the *ad hoc* development of the portfolio is to some extent as a result over the changing nature of funding streams. Also under the fEC model (once it is properly understood that it is operating in such a way to make things sustainable) it should be made clear what needs to be funded with significant Research Council/Funding Council contributions directly to the equipment.

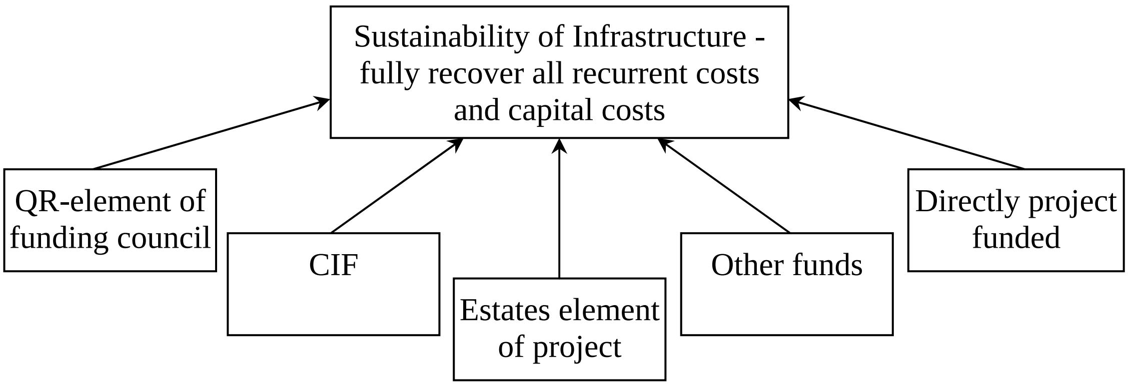
Potential funding streams include:

Estates costs – the guidance on estates costs has clearly allowed the recovery of all costs associated with equipment, including depreciation. Given how long ago some equipment was funded, such as under JIF and early rounds of SRIF, there should be some data for equipment (say NMR consoles and probes) now probably written off in the accounting sense and is approach the end of its practically useful lifetime, on how well the sustainability has developed for that equipment and any potential gap in sustainability from this source.

Capital investment fund (CIF) – The research element of such funding (RCIF) is to contribute to the long-term financial sustainability of the research activities of HEIs which includes the physical infrastructure that supports them. Although there is no direct connectivity between funding streams this is one of the sources that is identified for the obligatory contribution to RCUK funded equipment in the range £10k to the Office Journal of the European Union (OJEU) threshold.

Quality-related (QR) element of Funding Council Resourcing – As part of the UK's very successful dual support system QR has to underpin many elements of the research infrastructure. This is particularly true for equipment that cannot be directly attributable to project funding, with all guidance explicitly including key pieces of equipment.

A Direct Project Cost – As an MRF or SRF, costs or part of the costs of a facility can be recovered via a directly allocated or incurred cost on a grant. This of course depends on being able to calculate this in a way that translates to a rate that allows sustainable recovery as a product of that rate and funded activity that is successful.



Although TRAC provides a framework that looks to recognise the costs for making a facility fully sustainable, having a completely standard model across all facilities is probably not possible as there are some differences in detail between institutions and what is loaded into the sustainability model for a facility. In developing sustainability models there needs to be clearer guidance on:

(i) Dealing with depreciation both in the sense of having a common model of building it into the fEC rates and then mapping this more explicitly to the income funding streams;

(ii) Understanding how space charges are included in facility costs – which often differs between institutions in the way it is factored into their management accounts;

(iii) Dealing with non-fEC funded costs (e.g. research students, internal recharging of own-funded research), especially identifying whether and where the funding to cover these costs are currently located in the system.

In looking at the recent funding of NMR equipment some universities were already drawing a clear distinction between 'workhorse' underpinning facilities that were vital to the more general health of the discipline and the really leading-edge instrumentation that might allow really novel research in a related area or for technique/application development of the technique itself. It is clear that within university planning there is increasing provision of funding for scientific equipment, both new and replacement, within the medium term capital funding streams of the university. For the 'workhorse' underpinning core facilities some universities/departments had already taken on responsibility for the replacement and upgrade from 'own' funds (although the exact definition of own funds is not clear). Although this is a call for each university to make, in the light of what central capital funding streams are likely to be available they need to make decisions about what they themselves are prepared to make provision for and some guidance as to expectations of Research Councils as to the division of responsibility would be welcome. As a guideline, given the lead already given by some universities, there seems to be a split developing between for solution NMR at 500 MHz and below that is underpinning a wide portfolio of research. This would seem to be falling under the heading of a well founded laboratory. This should go into the capital planning of the HEI as opposed to being the expectation that this is specifically eligible for grant funding.

There should always be the opportunity for bids for equipment that is central to the research (i.e. that associated with a specific research proposal or centre of excellence that stands up to international standards) or where there is a need on the national level for provision of a facility to where the scale of investment is well beyond what a single HEI or even group of HEIs can be expected to provide. There are several examples of UK groups which are internationally leading in particular aspects of technique development. The 'National Facility' concept is exemplified by the High Field Solid State NMR Facility at Warwick which provides a 'free at the point of access' resource for the whole of the UK community. Given the pressure on funding, especially capital it is imperative for such facilities that they reconcile the funding in terms of the quality of the science they enable and having very robust mechanisms in place to check this, especially once they have been operationally for some time. The worth of a facility should be judged as a combination of utilisation, oversubscription by international standards along with quality of the outputs and impact of the research. For strategic equipment bids guidance as what a reasonable 'university contribution' was requested. Although there are no hard and fast expectations a commensurate contribution depending on the balance of research confined only to the researchers of that university to the creation of a facility/broader community element. A contribution would reflect that various funding council streams (e.g. QR, CIF) are part of the dual support of research which explicitly includes the provision of infrastructure for research and would not otherwise be possible for that university/group without the provision of that support.

4.2 Broader Sustainability Issues

At a practical level there are several other aspects of sustainability that could be considered. These mostly centre on the magnet. Magnets have long lifetimes, in excess of 30 years if they are well looked after. However technology (other than the availability of ever higher magnetic fields) has moved on in two crucial aspects, namely the development of shielded magnets producing greatly reduced magnetic footprints and hence space requirements of the magnetic fields. Secondly, magnet design in terms of the loss of cryogens have become very much more efficient meaning the hold times (times between refills) has greatly increased thereby reducing a central running cost. However the long lifetime of magnets has meant that since there is often no imperative to replace them, old design magnets have tended to be kept. Although a significant capital outlay, the efficiency gains in replacing magnets could result from the space gains along with the reduced cryogen consumption. So encouragement to HEIs to more proactively seek to replace older unshielded magnets should be considered.

The importance of installing more efficient magnets has been increased through the problems associated with the shortages of supply helium and noting the very real worry about how this could seriously affect the availability of helium for NMR and other scientific research. These would be a direct recurrent cost saving, as well as a strategic case for decreasing helium usage through magnet design. Surprisingly few universities have instituted helium recycling associated with NMR facilities. The economic case for recycling helium is still probably marginal. However there are two clear cut elements of a case for encouraging recycling helium including (i) improving resilience to issues with supply (i.e. when fewer litres have to be externally sourced), and (ii) there is the conservation of a finite resource. In keeping with universities being good model citizens in their social and corporate responsibility an aim to be as helium-neutral as possible would send a good signal. Given that the financial case is marginal only four universities either have or will in the coming year significantly recover their helium associated with NMR. Several universities mentioned that during the medium term that such recycling was going to be considered. It is a good time to re-examine this approach as new alternative cryogenic recycling technologies are becoming more widely available (e.g. conventional Joule-Thomson liquefaction vs closed cycle cold finger technology), EPSRC should consider incentivising use of more efficient magnets and installation of recovery systems.

5. Equipment Sharing, Efficiency of use and Strategy Development for NMR Infrastructure

The survey revealed that in most cases NMR spectrometers were heavily used, in most cases 24/7. Where NMR was used as a facility, as opposed to a primary research instrument, for standard experiments open, user programmed access is widely practiced, with good use made of robotic sample changers for walk-up access. Hence for the majority of spectrometers there was >80% usage. It emerged from the submissions from universities that under EPSRC Impact awards there are several projects looking at the more efficient use of such experimental resources through more automated and planned work flows. It seems that as there are several parallel projects in this area, once there are outcomes from these projects pooling what has been learnt and taking the best outcomes for more widespread use would be a good outcome for the sector.

Another area where there has been clear progress was in the development of groups of universities where there are commitments to examine asset sharing and the sharing in strategic assets when it was over and above the level what was needed as local day-to-day access. There is a view that real sharing is only likely to be considered when the equipment is regarded as beyond the reach of a single bid/institution, but there was an acknowledgement that this did depend on the institutional perspective. Signals of this change of behaviour was in shared asset registers, joint identification of necessary large scale investments across the group of institutions and even under the Core Capability for Chemistry Research call (11/12) two groupings put in *single* bids. Groupings that emerged as collaborating to some extent under asset sharing are:

Bath-Bristol-Cardiff
Eastchem (Edinburgh, St Andrews)
M5 (Birmingham, Leicester, Loughborough, Nottingham, Warwick)
N8 (Durham, Lancaster, Leeds, Liverpool, Manchester, Newcastle, Sheffield, York)
SES (Cambridge, Imperial, Oxford, Southampton, UCL)
Westchem (Glasgow, Strathclyde)

It was also interesting to see that linked to several of these consortia were then further relationships to either smaller or less research intensive institutions to present on a more formal footing access to key infrastructure that it would be unlikely that less research intensive HEIs could individually provide. The recently published EPSRC-funded report 'Sharing for Excellence and Growth'[6] noted there needed to be a balance as to what was locally available and that which could really be shared. Although sharing of highly specialised equipment was always possible, an estimate was made that there was likely to be a financial threshold in the window £200-500k where such sharing becomes more likely. These groupings or even wider groups coordinated procurement certainly enables more efficient use of resources. This is often greatly in the interests of HEIs, provided that any geographically distributed processes can ensure that individual researchers have their particularly specification needs catered for in detail. Such processes do not work well with very short procurement times related to requirements of rapidly needing to spend specific funding streams, which can only reduce the value for money which it is possible to obtain. RCUK with their considerable capital funding streams might want to consider what more active role they might play in procurement to ensure the best value for the public purse. To encourage sharing, ensuring that full costs of sharing (e.g. coordinating access) are met from funders was suggested. Although tighter capital funding can be seen as a driver of some of these changes there are undoubtedly positive benefits to performing top class research which is intimately connected to leading-edge research equipment.

6. Key Findings and Recommendations

6.1 There was a clear recognition that there is a direct connection between the provision of world-leading equipment and the ability to maintain the UK's position in producing world class research and that NMR is one of the key techniques.

6.2 Significant reassurance can be provided that through automation and efficient operation that very high utilisation rates are already being achieved across much of the NMR equipment base.

6.3 Behaviour change of HEIs with respect to capital infrastructure is already demonstrable with the provision of comprehensive searchable databases and groupings of universities sharing strategies for the joint provision of leading-edge equipment.

6.4 A review should be urgently undertaken of the data now fEC has been operating for a few years just how well recovery is working and making facilities sustainable.

6.5 Clear guidance as to the intended purposes of funding streams could be provided and how it is envisaged they are combined to delivery sustainability of equipment. There should also be clarity as to where it is anticipated that non-fEC activity (particularly PhD students) is funded from.

6.6 In improving efficiency of NMR EPSRC should consider incentivising upgrades to more shielded magnets and the installation of helium recovery systems associated with NMR facilities.

6.7 In discussion with the community clearer understanding of what capital funding is the responsibility of the HEIs and what is really eligible for Strategic Equipment Funding. On the basis of the evidence provided here it would seem that spectrometers ≤ 500 MHz for solution and ≤ 400 MHz for solids that are there as departmental/faculty/university facilities to underpin a large range of projects and part of the general laboratory infrastructure should be funded by the HEIs[7].

[6] N8 Report 'Sharing Excellence for Growth' July 2012, www.n8research.org.uk

[7] Currently to encourage upgrade to 600 MHz in such facilities these should be regarded as eligible for Strategic Equipment Funding

6.8 Strategic equipment should be identified with specialist capability for the UK of with really leading-edge facilities across groups of HEIs or UK wide.[8]

6.9 There is an urgent need for significant capital investment to address real weaknesses in comparison with our overseas competitors which has clearly been identified here as:

(i) Solution and solid state NMR provision at 700 MHz and above;

(ii) The provision of a commercial UK DNP facility, preferably at 600 MHz.

6.10 EPSRC should energise an RCUK discussion urgently to consider the approach to funding the NMR infrastructure at 1 GHz and above so the UK can remain competitive.

7. Conclusions

For the first time the scale of experimental provision across the majority of the HEI physical sciences base for a key experimental physical technique has been understood. NMR is very much seen as both a key underpinning technique and as a research topic in its own right. The utilisation rate of the current equipment base looks good and there is demonstrable progress in equipment sharing and joint development of strategies between HEIs. The funding of such capital infrastructure is complex and clarity over both the intended contribution of different funding lines towards sustainability and where the shortfall from non-fEC funded activity is expected to be funded from would be helpful. With the current Strategic Equipment Fund a suggestion has been made of what should be regarded as 'eligible' and also what looks to have the highest strategic importance for the UK community. It is absolutely clear that provision of higher field spectrometers and of a national open access DNP facility should be major strategic priorities and these will require significant new capital investment. The information that has been forthcoming from this survey strongly suggests that it would be worthwhile to undertake similar surveys in other widely used experimental techniques by the sciences within HEIs.

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Mark E. Smith, Lancaster, January 2013

[8] The most difficult case to deal with is equipment associated with specialist groups. However these could be seen as being clearly important as underpinning the strength of the expertise base (as opposed to a facility or service) and hence strategically important.