

UK National Crystallography Service Biannual Report 1

Period covered: 01/05/2010 – 03/10/2010

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1. Preface

In February 2010 the University of Southampton was successful with a tender bid (EPSRC Reference RCUK/D/EPSRC/Facilities/XRC/10 ; OJEU reference 002996- 2010) to host the UK National Crystallography Service (NCS). For context, an overview of the tender response is provided as Appendix 1. Service provision commenced on 1st May 2010 for a period of 5 years and the contract agreement defining the Service Level Agreement and Key Performance indicators was signed in late August 2010. The agreement (and indeed the original tender notice) stipulates that the NCS will be 100% operational by 1st May 2011 i.e. a year after commencing service provision and providing a 'ramping up' period. This is therefore the first biannual report under the agreement – this has two implications: a) the agreement was not signed until the end of August 2010 and this report is being compiled at the end of September 2010 – we consider this to be a working format (detailed strictly according to the schedules in the agreement) during the first year ramping up phase ; b) as part of the ramping up phase an entirely new electronic management and reporting system is being designed and implemented – this will be tailored to the reporting requirements of the contract, however there are some interim recording measures in place during the transition period. We therefore request feedback from EPSRC and the MAP as to the form and content of this report.

2. Operation and Logistics

A. Overview of service use

The NCS is currently going through a period of transition. The previous phase was operated under a 6 month extension to a 3 year research grant. Given the uncertainty of the future of the NCS (both existence and then funding and provider), it was decided to extend all allocations from the final formal round on a pro-rata basis until the end of the extension. The tender award to Southampton resulted in a contract being drawn up and derivation of a new set of Key Performance Indicators. There is therefore a mismatch between the old and the new processes and the data (and more importantly the recording of that data) to be provided for reporting purposes. The performance data are therefore in a period of transition and it should be noted that a comparison with previous allocation periods is not always possible or meaningful. It should also be noted that the period against which we are reporting is 5 months (due to the timing of the start of the contract and the timing of the reporting).

On the whole, the number of active users is considerably less than we would normally expect – this is most certainly due to the uncertainty of the future of the NCS this year and we have spent considerable time informing users who we have not heard from in some time that the NCS is still fully operational! That being said, the number of samples investigated in Southampton and at Diamond, is on a par with normal expectations. The number of samples waiting examination and outstanding is particularly high – this is wholly due to the increasingly unreliable nature of the old instrumentation base we are using, where repairs take a considerable time to perform.

B. Staff

The Southampton-based staff, Peter Horton, Graham Tizzard, Mateusz Pitak and Sarah Milsted have all had their contracts extended (after numerous interim contracts). These staff now take on expanded roles in order to develop their personal research careers and also to enhance the quality and diversity of research being conducted by the service. The organogram in appendix 1 indicates the areas of research expertise that individual members of staff will build on and hence feed back into the NCS. It is important to note here that Sarah Milsted has moved on from a simple sample handling position (at 0.1FTE) to a considerably more responsible role coordinating publicity and liaison, as well as administering the operation of the NCS (Sarah will be supervising an undergraduate project this year). The appointment of the Diamond member of staff to provide the synchrotron service is an ongoing process. A considerable number of very high quality applications were received by the deadline of 20th August – the appointment panel (Simon Coles, David Allan & Harriott Nowell) met in early September and interviewed 7 shortlisted candidates. An offer has been made and is being processed through Diamond HR system.

C. NCS Synchrotron component

Diamond Light Source Ltd (DLS) is to be subcontracted to provide the synchrotron component of the NCS, as per an outline provided by DLS to all tender bidders. A subcontract agreement outlining this relationship is currently in the final stages of being drawn up. As part of this relationship, a member of the NCS team will be based at and employed by DLS – interviews for this PDRA post were conducted in early September 2010 and an offer has been made. It is expected that this member of the team will be in post before the end of the year.

During AP7 5 days (15 shifts) were worked during the timeframe of the NCS tender i.e. since 1st May. This beamtime was a residual from the previous NCS grant. AP8 time (6 days, 18 shifts) was awarded at discretion of Diamond Director of Physical Sciences, due to the outcome of the NCS tender process not being known at the time of application and work commenced with 1 day on 1st October 2010. An application for 2-year programme mode access (Block Allocation Group, BAG, for AP9-AP12) commencing on 1st April 2011 was submitted on 1st October 2010.

D. Review of user complaints/disputes and resolutions

There have been no complaints reported to either the NCS Director or Head of Service and therefore no complaint or dispute resolution has been initiated.

E. Equipment- Technical Issues

The current equipment base consists of two diffractometers (generator 13 years old, goniometers 13 and 9 years old, and detectors 5 and 9 years old) and nitrogen temperature cryogenic equipment (two non- liquid nitrogen cryostats 4 years old). As expected of equipment this age there are numerous failures which are not preventable by routine maintenance. The following issues have arisen in the reporting period.

Diffractometers

- 2 filament changes (downtime 2 days each)
- 1 Ferroseal change (with 2 week downtime) replaced after just over 6 months operation.
- Various small components replaced on computers and ancillary equipment to keep them working (overall downtime 3 days)

Cryogenic devices:

- One returned briefly to Oxford Cryosystems for repair due to a faulty seal(downtime 5 days)

F. Sample Issues

The use of Mitegen pips, which are an industry standard, with magnetic bases is now normal working practice. The continuing problem of partially completed submission forms with sample related information missing (such as solvent/air sensitivity, melting point of crystals) has led to incorrect storage of samples and initial crystal selections having to be aborted.

G. Data Processing Issues

The data processing issues that have arisen since the beginning of the new NCS contract in May have mainly been related to Southampton personnel taking over the data collection and processing for the synchrotron component of the service. At Diamond Light Source (DLS), this is carried out using Rigaku CrystalClear software and initially none of the team were familiar with its use, however this has now been rectified by a combination of self-teaching and Rigaku support (Claire Wilson tutorial day).

There have also been issues with the Twinsolve module of CrystalClear, resulting in severe difficulties processing data from twinned crystals collected at DLS. This issue has recently (21.09.10) been resolved with the help of Rigaku technical support staff (Ken Yates).

We have redefined the data which is sent to a user on completion of full structure determinations and data collection only services. This has been done to clarify the difference between the two levels of service, making it easier for prospective users to identify which service they require and to set up the correct expectations of the service provided.

There have been no further data processing issues for this reporting period.

3. Community Activity

A. Training and Outreach

The NCS has hosted 3 visits since May. Each visit was tailored to the visiting group but each included a tour of the facilities, meeting the team and sessions with a crystallographer illustrating the technique and any special areas of interest to the group.

- Roman Kresinski (Kingston University) with 3 members of his research group
- Ben Le Reverand (Birmingham University) with 1 student
- Mike Cartwright (Cranfield University) with 1 colleague

We have also continued to take part in University of Southampton Open Days.

We have made contact with a number of groups taking part in outreach activities, including the University of Southampton and RSC regional groups. We are in the process of exploring outreach opportunities with these and other groups. We are particularly keen to contribute to next year's International Year of Chemistry celebrations.

B. Publicity

The NCS has produced flyers for distribution. There are two versions of the flyer, one targeted at institutions where there are no single crystal facilities and one which details our more advanced services for those with in house facilities. A spread sheet has been compiled listing department contacts, interested persons, previous and current users, this list will be constantly added to enabling us to contact potential users quickly and easily. Over 600 flyers were distributed publicising the service, and this first call.

As well as being sent to department contacts flyers were distributed at the Southampton Supramolecular Chemistry Symposium in July and we will be looking to distribute publicity at conferences more widely in 2011.

The service has been completely rebranded with a new logo, website and style. The website will be developed heavily in the upcoming months to increase the amount of information available to users and interested persons.

Standardised materials such as PowerPoint slides and wording for acknowledgements will be drawn up to make it as easy as possible for users to acknowledge the service, and for the service to be quickly and easily recognised.

4. Preview of next period

A. Preview of availability over next 6 months

The next 6 months (NCS period Nov-April) is going to be rather fluxional for the NCS. A new laboratory must be constructed, including order of instrumentation, identification of location, repurposing of space and delivery, construction & commissioning of equipment. During this work, the NCS will continue to operate (eventually in parallel to the developing new laboratory) on its current (13 year old) instrumentation. The current equipment is no longer produced by the original manufacturer and support is becoming expensive and difficult to provide. We will continue to operate the machine, but wish to point out that there could be a potentially fatal or prohibitively expensive breakdown. Phasing in of new instrumentation is dependent on delivery times, more details about this will be communicated as they become available.

There is no foreseen period, apart from the University of Southampton closed days over the Christmas break, when the NCS will not be available. Availability of the diffractometers is dependent on up time of current instrumentation, although there is no scheduled servicing due in the next six months, the instrumentation is reaching the end of its life and unexpected downtime may be an increasing factor until the new equipment is commissioned.

Thursday PM and weekends will continue to be unavailable for the service as this is scheduled department time. The service and department continue to have good lines of communication meaning time not utilised by either party in their scheduled hours is made available to the other. There is also room for negotiation should the service have a short term need for additional hours.

B. Preview of maintenance over next 6 months

There is no major service work scheduled, however filament will need to be replaced (approximately every 2 months). For this reason a pack of new filaments have to be bought from Bruker, before new equipment will be delivered and set up. The vacuum pumps should be swapped when next filament is replaced.

C. Preview of upgrade over next 6 months

In the next few days, the NCS will negotiate with the successful bidder to the equipment tender, inform the unsuccessful bidder and enter the 'Alcatel' period (15 days), where the outcome of the process may be contested. We therefore expect to formally place an order before 22nd October 2010. Both bidders fulfilled the criteria of the tender specification and the evaluation process was very thorough with a close outcome. The new instrumentation will be delivered, constructed and commissioned within the timeframe of the upcoming period. This will also involve identification and repurposing of space for a facility to house the new equipment. The current equipment base will continue to be operated during this whole process. Further details on the progress of this process, if available, will be provided at the MAP meeting in Southampton on 7th October 2010.

D. Preview of developments in x-ray crystallography techniques

NCS will purchase a new cold-stream mounting device (as detailed in the tender) and construct a new schlenk line in the new laboratory. We also intend to source a light microscope and additions to the thermal analysis support laboratory (depending on the outcome of the equipment tender negotiation process).

E. Preview of developments in x-ray crystallography technology

A new detector technology is becoming available for use in a number of diffraction-based techniques – a complementary metal oxide semiconductor (CMOS) hybrid-pixel technology, which operates in single-photon-counting mode. The very rapid detection rate and (lack of) read-out time mean that image collection will be considerably reduced (minutes rather than hours). An example of this is the Pilatus detector from Dectris and the NCS is in discussion with potential equipment suppliers regarding the implementation of this technology on its instrument base.

Appendix 1: KPI Data (All data for 01/05/10 – 03/10/10)

Number of NCS Users (active)	39
Number of NCS Projects	44
Availability of facility for NCS use (days)	107
Actual equipment uptime and use of facility by or for NCS	90
Number of NCS samples processed	273 (not including synchrotron samples)
Number of NCS data collections performed	221
Number of Full structure determinations performed	52
Number of synchrotron samples	69
Number of NCS samples outstanding	184
Waiting for examination	53
Processing	96
Waiting for return to users	35
Number of User data sets that were completed within 1,2,3, and >3 attempts – we are currently unable to report against this point.	
Number of User complaints received	0
Number of NCS research outputs	26
Number of NCS users of the training programme	8
Number of samples classes as routine or difficult – we are currently unable to report against this point.	

Appendix 2: Benchmark statistics

Benchmark 1

The time from arrival of a sample to logging in and informing a User of receipt will be within 2 working days for all samples

Level of samples which achieved this benchmark 100%

Benchmark 2

The time a sample is in the queue from logging in a sample to the first examination will be within 10 working days for 80% of high priority samples, within 20 working days for 80% for medium priority samples and within 30 working days for 80% of low priority samples.

Level of samples which achieved this benchmark H- 95%

M-96%

L- 100%

Benchmark 3

The time a sample is in the queue from examination and first communication of the outcome will be provided within 5 working days for 80% of all samples

Level of samples which achieved this benchmark 89%

Benchmark 4

The time between the first communication of the outcome of a data collection and the provision of a final result will be within 5 working days for 80% of all samples.

Level of samples which achieved this benchmark 85%

Appendix 3: Publications List

Arising from use of the Southampton Facility

1. I. Afonina, P. J. Skabara, F. Vilela, A. L. Kanibolotsky, J. C. Forgie, A. K. Bansal, G. A. Turnbull, I. D. W. Samuel, J. G. Labram, T. D. Anthopoulos, S. J. Coles and M. B. Hursthouse, *Journal of Materials Chemistry*, 20, 1112-1116.
2. M. A. Beckett, E. L. Bennett, P. N. Horton and M. B. Hursthouse, *Journal of Organometallic Chemistry*, 695, 1080-1083.
3. M. A. Beckett, P. N. Horton, M. B. Hursthouse, D. A. Knox and J. L. Timmis, *Dalton Transactions*, 39, 3944-3951.
4. M. A. Beckett, P. N. Horton, M. B. Hursthouse and C. Pszolla, *Acta Crystallographica Section E-Structure Reports Online*, 66, O833-U2327.
5. M. A. Beckett, P. N. Horton, M. B. Hursthouse and J. L. Timmis, *Acta Crystallographica Section E-Structure Reports Online*, 66, O319-U2063.
6. B. J. Coe, S. P. Foxon, E. C. Harper, M. Helliwell, J. Raftery, C. A. Swanson, B. S. Brunschwig, K. Clays, E. Franz, J. Garin, J. Orduna, P. N. Horton and M. B. Hursthouse, *Journal of the American Chemical Society*, 132, 1706-1723.
7. C. Dawson, P. N. Horton, M. B. Hursthouse and S. L. James, *Crystengcomm*, 12, 1048-1050.
8. A. P. Dobbs, S. J. J. Guesne, R. J. Parker, J. Skidmore, R. A. Stephenson and M. B. Hursthouse, *Organic & Biomolecular Chemistry*, 8, 1064-1080.
9. J. R. Galan-Mascaros, E. Coronado, P. A. Goddard, J. Singleton, A. I. Coldea, J. D. Wallis, S. J. Coles and A. Alberola, *Journal of the American Chemical Society*, 132, 9271-9273.
10. G. Gasser, J. D. Carr, S. J. Coles, S. J. Green, M. B. Hursthouse, S. M. Cafferkey, H. Stoeckli-Evans and J. H. R. Tucker, *Journal of Organometallic Chemistry*, 695, 249-255.
11. O. O. Guven, M. Bayraktar, S. J. Coles and T. Hokelek, *Acta Crystallographica Section E-Structure Reports Online*, 66, O1246-U1224.
12. O. O. Guven, M. Bayraktar, S. J. Coles and T. Hokelek, *Acta Crystallographica Section E-Structure Reports Online*, 66, O959-U3383.
13. O. O. Guven, H. Tahtaci, S. J. Coles and T. Hokelek, *Acta Crystallographica Section E-Structure Reports Online*, 66, O107-U1978.
14. M. Iglesias, D. J. Beetstra, K. J. Cavell, A. Deryisi, I. A. Fallis, B. Kariuki, R. W. Harrington, W. Clegg, P. N. Horton, S. J. Coles and M. B. Hursthouse, *European Journal of Inorganic Chemistry*, 1604-1607.
15. L. Kyros, N. Kourkoumelis, M. Kubicki, L. Male, M. B. Hursthouse, Verginadis, II, E. Gouma, S. Karkabounas, K. Charalabopoulos and S. K. Hadjikakou, *Bioinorganic Chemistry and Applications*.
16. B. J. D. Le Reverend, P. J. Fryer, S. Coles and S. Bakalis, *Journal of the American Oil Chemists Society*, 87, 239-246.
17. E. Martin, W. Clegg, R. W. Harrington, D. L. Hughes, M. B. Hursthouse, L. Male and S. J. Lancaster, *Polyhedron*, 29, 405-413.
18. L. Martin, P. Day, P. Horton, S. Nakatsuji, J. Yamada and H. Akutsu, *Journal of Materials Chemistry*, 20, 2738-2742.
19. L. Martin, P. Day, S. Nakatsuji, J. Yamada, H. Akutsu and P. Horton, *Crystengcomm*, 12, 1369-1372.

20. L. Martin, P. Day, S. Nakatsuji, J. Yamada, H. Akutsu and P. N. Horton, *Bulletin of the Chemical Society of Japan*, 83, 419-423.
21. G. J. McEntee, P. J. Skabara, F. Vilela, S. Tierney, I. D. W. Samuel, S. Gambino, S. J. Coles, M. B. Hursthouse, R. W. Harrington and W. Clegg, *Chemistry of Materials*, 22, 3000-3008.
22. G. Mirri, S. D. Bull, P. N. Horton, T. D. James, L. Male and J. H. R. Tucker, *Journal of the American Chemical Society*, 132, 8903-+.
23. J. L. Nicholls, S. E. Hulse, S. K. Callear, G. J. Tizzard, R. A. Stephenson, M. B. Hursthouse, W. Clegg, R. W. Harrington and A. M. Fogg, *Inorganic Chemistry*, 49, 8545-8551.
24. M. M. M. Santos, N. Faria, J. Iley, S. J. Coles, M. B. Hursthouse, M. L. Martins and R. Moreira, *Bioorganic & Medicinal Chemistry Letters*, 20, 193-195.
25. L. A. Smyth, T. P. Matthews, P. N. Horton, M. B. Hursthouse and I. Collins, *Tetrahedron*, 66, 2843-2854.
26. J. Spencer, B. Z. Chowdhry, S. Hamid, A. P. Mendham, L. Male, S. J. Coles and M. B. Hursthouse, *Acta Crystallographica Section C-Crystal Structure Communications*, 66, O71-O78.

Publications arising from NCS use of DLS

1. Songjie Yang, Andrew C. Brooks, Lee Martin, Peter Day, Melanie Pilkington, William Clegg, Ross W. Harrington, Luca Russo and John D. Wallis, *Tetrahedron*, Volume: 66, Pages: 6977-6989
2. William Clegg, Ross W. Harrington, Michael North, Francesca Pizzato and Pedro Villuendas, *Tetrahedron: Asymmetry*, Volume: 21, Pages: 1262-1271
3. William Clegg, Ross W. Harrington, Michael North, and Pedro Villuendas, *Journal of Organic Chemistry*, Volume: 75, Pages: 6201-6207
4. G. J. McEntee, P. J. Skabara, F. Vilela, S. Tierney, I. D. W. Samuel, S. Gambino, S. J. Coles, M. B. Hursthouse, R. W. Harrington and W. Clegg. *Chem. Mater.*, 2010, 22, 3000-3008.
5. J. L. Nicholls, S. E. Hulse, S. K. Callear, G. J. Tizzard, R. A. Stephenson, M. B. Hursthouse W. Clegg, R. W. Harrington and A. M. Fogg. *Inorg. Chem.*, 2010, doi: 10.1021/ic101145p.
6. H. V. Goulding, S. E. Hulse, W. Clegg, R. W. Harrington, H. Y. Playford, R. I. Walton and A.M. Fogg., *J. Am. Chem. Soc.*, 2010, doi: 10.1021/ja104636x. Featured on cover of JACS (publication date Oct 6th 2010) and as a highlight on the Diamond website.
7. FJ McInnes, NG Anthony, AR Kennedy & NJ Wheate., *Org. Biomol. Chem.*, (2010), 8, 765-773.
8. D. L. Holden, H. V. Goulding, J. Bacsá, N. G. Berry, N. Greeves, R. A. Stephenson, W. Clegg and A. M. Fogg, *Crystal Growth and Design*, 2010, Submitted.
9. G. McEntee, F. Vilela, P. J. Skabara, T. D. Anthopoulos, J. G. Labram, S. Tierney, R. W. Harrington and W. Clegg., *J. Mater. Chem.*, 2010, Submitted.

Appendix 4: Tender Overview

The National Crystallography Service (NCS) at Southampton - a 10 year vision

This tender seeks support for a new UK NCS, to be operated within the Southampton Centre for Single Crystal Diffraction, co-funded by the University of Southampton and incorporating a streamlined conduit to synchrotron facilities at DLS. It will provide the UK science research community with access to a world-leading facility, supporting structural science in all chemical, biological and physical areas, and capable of tackling problems that may not be amenable to study using facilities available in most local research laboratories. In this rich environment the combined facility will continue the tradition established by the current NCS to seek out and activate interactions with equipment manufacturers and with world-renowned experts in other laboratories in the UK, in Europe and other continents, to ensure continuing contact with cutting edge technology and methods. The Facility will operate in an **efficient and highly professional** manner and will demonstrate **best practice** and **technological innovation** in the subject, and make the acquired expertise openly available to the UK research community.

The proposed 'next generation' NCS will build upon **three decades of proven track record** in advancing the technique and turning that into service delivery. It will provide new, state-of-the-art instrumentation, and will continue to benefit from the considerable experience and excellent technical expertise of [Drs S. J. Coles, M. E. Light](#) and [P. Horton](#) in running the current, highly respected, NCS (originally under the Directorship of Prof. M. B. Hursthouse), ensuring that it meets all the needs of the crystallography community across the UK for the foreseeable future.

This proposal for the new NCS will bring **brand new facilities**, operating at the forefront of crystallographic methods, capable of meeting the new challenges emerging for chemists, biochemists and materials scientists, including the areas of macromolecular, supramolecular and protein crystallography. The instrumentation will be co-located within the School of Chemistry, and the NCS staff will work closely with the equipment manufacturers towards further developing the instrumentation to maximise its utility to the community.

Whilst continuing to provide means of structure characterisation on user-supplied samples up to and including the most extreme problem samples, technique development in the application of diffraction and other experiments to probing more advanced or applied structural aspects will also feature strongly in the provision to users. Priority areas for such experiments are charge density determination, variable temperature work, phase transition characterisation, structure-property relationships, structural systematics, understanding polymorphism and crystal growth, and in further developing innovative methods for data management and use, including seamless linking to intelligent software for interpretation of structural features and for follow-on theoretical calculations to derive properties from/of crystal structures. These also build upon existing strengths and will be extremely beneficial to the UK user community.

The facilities available in the proposed NCS will be made possible in part through the considerable financial contribution from the UoS (£500k of which £400k will be used for diffractometer purchase, whilst £100k will be used to construct a crystallisation facility to which the NCS will have unhindered access), a demonstration of the unequivocal support for this vision and in recognition of its close synergy with the University's own research ambitions in structural science. The UoS is committed to further strengthening its research base in structural science through the imminent appointment of a senior structural biologist with expertise in protein/ macromolecular crystallography who will conduct diffraction experiments in the Centre. This collaboration will provide a wide-ranging capability for NCS and local users in a cost effective manner through a carefully and equitably managed shared equipment base.

A key operational objective for the new NCS will be to increase its profile and highlight the new capabilities among the existing and potential new (multidisciplinary) user community, to maximise the benefits to the UK research community. This will be led by [Prof. P. A. Gale](#) (Deputy Head of School), who will bring a **'user'-based perspective** to the service on one hand (as well as a high international profile and reputation in structural supramolecular chemistry in collaboration with the current NCS staff), while aligning well with the Senior Management in the University to ensure the priorities of the new NCS are fully considered at the highest level.

Training and outreach will feature strongly in the new NCS, ensuring users receive access to specialised training in crystallography, while also providing suitable advanced training and CPD for its staff. In recent years, public engagement and outreach to school students have been a growing element of the NCS activities at Southampton, and will be provided e.g. through demonstrations, school visits, hands-on workshops at science fairs, web-based activities and remote access.

Overview of Service Level

The proposed facility will form the Southampton Centre for Single Crystal Diffraction located within the School of Chemistry, and includes a £500k contribution towards the new equipment from the University of Southampton (also see attached Letters of Support in **Appendix 2** confirming the university's commitment). The UoS contribution is to be split into £400k for diffractometers and £100k for a crystallisation facility.

The tender offers two levels of service, reflecting expected levels of throughput required by the UK research community over the next ten years. The higher level will enable the NCS to meet all targets identified in the call document, including scope for strong future developments. The lower level will meet the baseline demand outlined in the tender document. The equipment resources specified are based upon our experience of likely sample types and numbers at two service levels for an increased throughput of small molecule single crystal structure determinations, a new capability to determine structures using copper radiation and fast turnaround access to synchrotron radiation. Full details of the bases and rationales for the two tenders and likely performance levels are provided in the detailed sections which follow this and accompanying overviews.

This service level offers the most flexible processing capability for a range of sample types, from very small crystals to crystals of large macromolecular samples including proteins. This will comprise:

- one state-of-the-art **very** high flux rotating anode Mo source equipped with two diffractometers (to be purchased new);
- one high flux Cu diffractometer (to be purchased new);
- continuing use of the existing twin KappaCCD rotating anode Mo source, until it clearly reaches the end of its operational life (now 12 years old and its continued use is a testament to the skills of the Southampton staff in attending to in-house maintenance), when the option will be available to reconfigure the ApexII detector (the most recent acquisition (2006) of this kit) on a new generator;
- providing seamless access to the very high flux synchrotron source at DLS

All new equipment will be supported by manufacturer service contracts for the five year period of the tender and routine preventative servicing will be undertaken by the staff within the scope of the contracts.

Additional facilities available for use to the NCS include:

- differential scanning calorimeter
- hot-stage video microscope
- polarising microscope
- 2 x Cobra; 3 x Cryostream cryostats
- optical microscopes
- vacuum line, dry box and low-temperature crystal mounting apparatus

Central to the facility will be the presence of highly trained technical crystallographic and data handling experts whose remit will be to provide an efficient and professional service that meets the needs of the UK user community, and will be led at the operational level by Dr Simon Coles.

Since the present NCS is hosted in Southampton, the transition will be very straightforward, with no requirement for transfer of sample handling or data records. Current users are already familiar with the processes and protocols for accessing the service, and the procedures will be transparent from the outset, hence allowing ease of access to new users. The application process and refereeing criteria will be openly available via the web-site.

The new Service will continue to operate with its current equipment on 'Commencement of Service', i.e. providing a baseline service from day one within the UoS; the synchrotron facility will be available from the beginning of AP7 (April). Following procurement and ordering, the new equipment will be installed and commissioned within approximately 8 months from notification of award of the tender.

The remaining considerations are the switch-over to the new instrumentation and introduction of the new capabilities of the NCS. A maximum period of one month will be required to transition to the new equipment, but we expect to maintain a baseline service even during the transition period. Full capability is guaranteed within 12 months from the start of the contract.

The new suite of diffractometers will offer a resilient base of instrumentation that will secure high levels of service into the future, underwritten by service contracts with the manufacturers. Several other contingencies have been factored in to ensure uninterrupted access to the NCS for users even in the event of a serious failure.

The NCS will work with EPSRC to derive a set of metrics and Key Performance Indicators and Service Level Agreements. Performance will be monitored internally by the Head of Service, with oversight from the Management Advisory Panel and EPSRC. Service level data will be published on the NCS web-site, allowing the NCS to demonstrate transparently the level of service offered to users.

Overview of Technical Capability

The present NCS is hosted in Southampton and has an extensive track record in innovating and delivering on all aspects of service provision over the last three decades and has established a highly professional set of processes and protocols. The new NCS will build on these to act as an example of best practice in many areas, but particularly playing to its strengths in innovating crystallographic instrumentation and service operation, dealing with the most difficult samples and data, data management and publication, eScience, upholding the quality of crystal structure data (through RSC checking activities) and excellence in research into focussed techniques such as structural systematics, charge density and variable temperature phase transition work.

The first area detector worldwide to be fully employed as a service tool for chemical crystallography was commissioned by the NCS and revolutionised throughput – nowadays all diffractometers for chemical crystallography have this technology. A few years ago the NCS also initiated the development of the first focussing mirrors for Mo radiation, which enabled a step change in the size and quality of crystals that can be examined in the laboratory. NCS was the first mid-range experiment-based facility to embrace eScience and we are now on the verge of a revolution in how data are managed, published and exploited.

The instrumentation that will underpin the NCS is to be sourced new and specifically for the task of operating a high throughput, service-oriented laboratory. The NCS has a long tradition in making such decisions and building the rapport with manufacturers that is essential to making bespoke mid-scale facility instrumentation work and that will enable a step change in what is possible. This same rapport is necessary for the on-going running of the equipment and for creating a showcase Centre that will be a driver, an early adopter or a tester of new innovations. A full Service contract is costed into this application to ensure upmost reliability and that the equipment still provides a platform for the proposed 10 year vision after this current funding period.

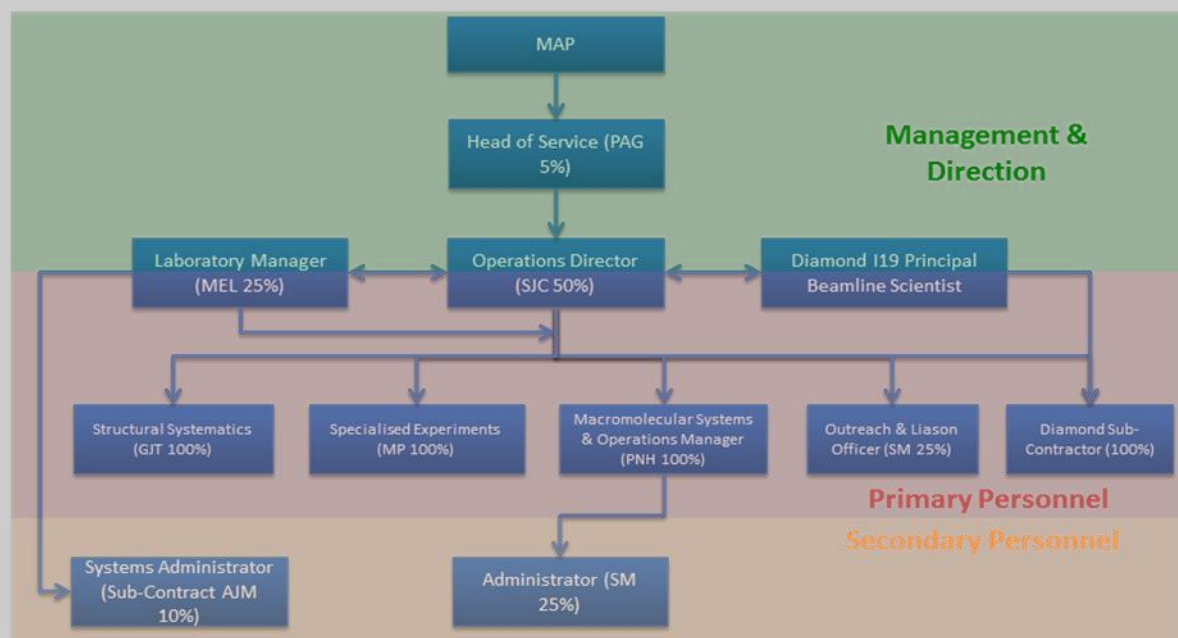
Priority areas for research are polymorphism, crystallisation and structural systematics, macromolecular work on both chemical and biological systems, charge density studies and the study of variable temperature phase transitions. Recognising that a crystal structure is more than a characterisation of a compound and that it is also a point in a very large dataset, the NCS will take innovative directions that provide added value to the data it generates. Building on strengths honed over two decades in generating, managing, examining and exploiting large families of data, the NCS will act as consultants, tutors or collaborators on structural systematics projects. Particularly, NCS will support and collaborate on the use of the program XPac and other related software in the field to analyse families of crystal structures and relate this to properties by means of crystal lattice and energetic calculations.

The NCS has been involved with the eScience programme right from its very outset and SJC has maintained a lead in this area from both service delivery and also research and development perspectives. SJC holds a number of grants in this area and will draw on all this expertise and the experience of the eScience research group to deliver a sample and data management system with a user interface that will demonstrate best practice and serve all the NCS requirements for the period of this tender and more.

Both SJC and MEL have long association with the NCS for some time. SJC has a proven track record from over 10 years of managing the NCS - from a record keeping and reporting perspective, from delivering results on challenging samples and according to prescribed quotas and also from providing new funding and direction. MEL moved from the NCS to become the School Crystallographer and has been responsible for the upkeep and running of all the diffraction equipment in the department (the NCS rotating anode with 2 diffractometers and 3 powder diffractometers). The NCS postdoctoral staff are experienced in both service crystallography and structural

chemistry research and have been highly trained (all at least second-term). They have individual research aspirations and experience and a proven ability to deliver in both service-based and research-based areas. For the last two years, the NCS team have been part of a consortium of reviewers responsible for maintaining the quality in RSC journal articles – this position involves a high degree of technical capability and an understanding of the responsibility for high quality results.

Overview of Staff and People



The NCS will operate a Management Advisory Panel (MAP), the Chair of which will be appointed (externally) by EPSRC and with representatives from different groups within the user community. The MAP will referee and prioritise the applications to use the NCS (the same mechanisms applying to all UK applicants), monitor performance related to SLAs and KPIs, and provide strategic direction.

The MAP and Head of Service are responsible to EPSRC. The Head of Service, Prof. P. A. Gale, is also Deputy Head of School, and will report internally to the School of Chemistry Senior Management Group. PAG has worked with the current NCS team over the last 11 years and has an excellent understanding of the needs of the service users. PAG has a high international profile in structural supramolecular chemistry (h-index 47, 40 years old, > 8000 citations, > 160 publications) and is a regular plenary or keynote speaker at meetings around the UK and internationally. PAG will actively promote the NCS at national and international meetings, and will work with the NCS staff and MAP to encourage new users to the NCS and to promote the new capabilities available through the service.

The Operations Director, Dr S. J. Coles, is co-director of the current NCS, with 18 years experience of service crystallography, in addition to maintaining a high profile in informatics and electronic management of data. He is active in developing new innovations in and applications of crystallography. He initiated development of focussing mirrors to increase radiation intensity, allowing study of much smaller crystals and higher throughput of samples. This technology is now included in many commercial diffractometers. Other major areas of study are in elucidating the mechanisms of phase transitions and systematic charge density studies on families of compounds (with Wakayama, Japan and NTU (with EPSRC funding)).

SJC already works closely with the Laboratory Manager (MEL) and Diamond I19 Principal Beamline Scientist, and will continue to do so to ensure streamlined access to and efficient usage of the synchrotron facilities; he will also line manage all the primary Service personnel. MEL will oversee technical operation of the equipment and ancillary systems. MEL also has long experience of service crystallography, and is extremely talented in solving 'difficult' structures. His primary role is Manager of X-Ray Diffraction in the School of Chemistry (75%). Within the NCS he

will provide technical and maintenance support, as well as supporting the service personnel in structure determination.

The other service personnel are Dr P. Horton (PNH), Dr G. Tizzard (GJT), Dr M. Pitak (MP). All of the core staff who will work on the Service are already in post, ensuring a rapid transition to the new NCS, and providing extensive experience of delivering a successful UK NCS. These staff are members of the RSC structure checking consortium led by SJC – this work is of great worth to the crystallographic community in ensuring that a high standard in crystal structure checking is maintained. SJC is working with the IUCr and RSC to bring all the RSC crystallographic checking under one umbrella, which would be coordinated from Southampton and would be considered to be a NCS activity.

The Diamond I19 Principle Beamline Scientist will be responsible for the line management of the Diamond beamline staff involved in the Service and coordinating the implementation of the Diamond Sub-Contract terms and conditions.

Training and continuous professional development will continue to be key considerations for all staff associated with the Service, both in the theory and practice of X-ray crystallography (including synchrotron based experiments) and in emerging new innovations associated with the field. They will also gain training and developing teaching skills at UG and PG levels, as well as in providing user training. All staff associated with the NCS will have a clearly defined line management structure and appraisal processes as would be appropriate for ECRs.

Emeritus Professor M. B. Hursthouse, founder of the NCS, continues to provide invaluable advice and direction. He holds the post of Emeritus Professor and will continue his research activities for the duration of the award period; he will act as a consultant for the NCS management through the Head of Service and as an advisor to the Operational Director on running matters.

Overview of Customer Interface

The interface between the NCS and its users is critical to its success and to ensuring that it is best able to respond to the existing and emerging needs of the research community. The service will deliver both data set acquisition and full structure determinations (publication-ready).

An administrative assistant employed on the service will provide the first point of contact for users and will be responsible for updating users on the progress of their samples throughout the service process. The SLAs and KPIs will be published on the service web-site, together with current performance metrics. The service will encourage visits from users when beneficial to either party in order to illustrate the range of facilities available, to provide specialist input into a particular structural problem, for 1:1 training purposes and during synchrotron data collections as appropriate.

Training opportunities will include data collection and structure determination, and will be delivered through a variety of means, including hands-on (1:1) experience, scheduled workshops for beginners and experienced users, on-line resources and video-conferencing facilities for remote users.

Promotion of the service will be through:

- (i) the service website detailing facilities, service level, procedures and contact details, EPSRC web-site, DLS web-site and the University of Southampton web-site;
- (ii) external presentations at national and international scientific conferences, synchrotron user meetings etc through the service staff and Head of Service;
- (iii) technical publications, newsletters and meetings e.g. BCA, IUCr, DLS, Durham Crystallography Course;
- (iv) promotional literature to be distributed widely across UK HEIs;
- (v) co-authorship/acknowledgement of the NCS in primary research literature (co-authorship normally for full structure solutions and specialist experiments; acknowledgement normally for data collection)

The NCS staff will promote crystallography and structural science to the wider community (public) through its website, Schools outreach (primarily through provision of activities, tours etc for events coordinated by the

University Outreach and Partnership Division and by the School of Chemistry's Outreach Coordinator), and through provision of public engagement activities e.g. National Science and Engineering Week.

The first point of interaction with the NCS will be through the MAP which will regulate facility access. The MAP will comprise a body of independent experts whose primary functions will be to set prioritisation levels and advise on strategic direction. Coupling of the NCS Administrator role with the appointment of an Outreach and Liaison Officer will provide a point of contact for all users and general public with the NCS and promote the building of a strong rapport. In addition the sample and data management system will have a user-facing interface that will provide seamless interaction with their data and sample or project information. This system will also empower users to manage, interact with and publish their data in full collaboration with NCS staff.