

Annual Report for EPSRC National Research Facilities

Facility: EPSRC National Crystallography Service

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Value Proposition

Crystal structure analysis is the dominant and most informative characterisation technique available and is a cornerstone underpinning cutting edge research in chemistry and related disciplines. The National Crystallography Service (NCS) provides structural characterisation support which crucially drives research across the range of disciplines performing chemical synthesis and materials characterisation. The NCS facility is amongst the most powerful and highest throughput of its type in the world. Building on this platform, its core service provides state-of-the-art structure characterisation, significantly beyond that found in home departments, for chemists, materials scientists and crystallographers in academia and industry.

Crystallisation or subsequent diffraction quality of a new compound is not predictable and so synthesis chemists need timely recourse to higher-powered facilities, but not for all their samples – thus making a centralised facility the only scalable and financially viable option. The ability to handle the most demanding samples in a University-based facility provides an effective screen for a follow-on synchrotron service. The NCS has regular access to the world leading I19 beamline at Diamond Light Source, making the use of this facility as efficient, cost effective and timely as is possible. Sample turnaround time is exemplary, meaning that this technique is often used to progress research, as well as producing the characterisation of its final outputs.

The NCS greatly enhances the reach of the technique by the in-situ study of dynamic solid-state systems at high temperature, pressure and in different gaseous environments. This underpins developments in areas of strength e.g., energy, carbon capture, functional and catalyst materials, but requires specialised equipment and significant experience to perform such experiments, often considered the preserve of the expert crystallographer. The NCS broadens the impact of these techniques by making them available to the wider chemistry community.

The NCS is a world leading facility and spreads its expertise by educating, facilitating, and empowering non-experts across the community, particularly in providing advanced training opportunities. It increases the levels at which structure characterisation can be carried out in the UK and enables a step change in accessibility of the technique to entirely new communities.

Scientific Excellence

Core Service Highlights

The NCS provides a state-of-the-art service for structure characterisation, significantly beyond that found in home departments, for chemists, materials scientists and crystallographers in academia and industry. It enables the UK to remain a world-leader in structural science, providing structural characterisation support which is crucial to drive research across the range of disciplines performing chemical synthesis. The NCS underpins cutting edge research e.g. progressing the drive towards a circular plastics economy is driven by Prof C Redshaw, Hull - we report 5 papers underpinned by NCS data on this topic, a particularly important one reporting more efficient catalysis in the formation of polyethylenes in Catalyst Science and Technology

(<https://doi.org/10.1039/D0CY01979H>). A recent review by Simon Coles in the 2020 issue of 'Structure and Bonding' (21st Century Challenges in Chemical Crystallography) entitled "Leading Edge Chemical Crystallography Service Provision and Its Impact on Crystallographic Data Science in the Twenty-First Century" extensively details the scientific excellence delivered by the NCS core service.

The exceptional level of publications outputs (see Publications section below) is testament to the scientific excellence both supported and driven by the NCS. In this reporting period 26 co-authored papers were published and this is supplemented by at least the same number of papers also arising from the data collection only service. Some publication highlights, selected from very high Impact Factor journals, during this period include:

Guest Binding Drives Host Redistribution in Libraries of Co(II)₄L₄ Cages (Angew. Chemie - Int. Ed - <https://doi.org/10.1002/anie.202004627>) - Work performed by the Nitschke group (University of Cambridge) investigated the guest-host binding capabilities of a number of Co(II) tetrahedral cages towards various anions. The service was used to obtain vital structures of the two separate cobalt cages, demonstrating the differences between the two with regards to anion binding. The NCS also collected a library of structures of co-crystals of the cages in various mixtures, via both in-house instruments and facilitated time at the Diamond synchrotron.

Tuning the anion binding properties of lanthanide receptors to discriminate nucleoside phosphates in a sensing array (Chem. Sci. - <https://doi.org/10.1039/D0SC00343C>) - Work performed by the Butler group (Loughborough University) synthesised a range of lanthanide complexes which were found to selectively bind nucleoside phosphate anions. It was demonstrated that the lanthanide complexes are excellent candidates for differential anion sensing in a high-throughput array format with huge implications for biomedical research and drug discovery. The data for the crystal structure of the original europium complex was obtained by the NCS and formed the basis of the publication.

Stable metal-organic frameworks with low water affinity built from methyl-siloxane linkers (Chem. Commun. - <https://doi.org/10.1039/D0CC01186J>) - Work performed by the Davies group (Imperial College London) led to the first examples of Zr/Hf-MOFs incorporating siloxane-based linkers. The resulting MOFs have very low water affinity without compromising their porosity which is hugely promising for potential applications in air purification and carbon capture. It was also demonstrated that the novel siloxane-based tetracarboxylic acid that formed the Zr/Hf-MOFs would also self-assemble into an interpenetrated supramolecular network. Datasets of both the self-assembled network and the Zr MOFs were obtained by the NCS and were imperative for the demonstration of the MOF porosity.

A Structurally Characterized Cobalt(I) σ -Alkane Complex (Angew. Chemie - Int. Ed - <https://doi.org/10.1002/anie.201914940>) - Collaboration between the Weller group (University of York, formally of the University of Oxford) and the NCS, produced a novel cobalt σ -alkane complex. Alkanes are typically poor ligands and are often displaced by solvents, making alkane complexes incredibly difficult to observe. By utilizing single-crystal to single-crystal gas/solid reactivity, the requirement for a solvent is removed allowing the σ -alkane complex to form. This is further discussed in the Advanced Techniques Highlights below. The NCS was instrumental in the development and application of this *in situ* gas cell experiment and will continue to work closely

with the Weller group in this area. The collaboration with Prof Weller is also the subject of a case study submitted with this report.

Uranium(IV) cyclobutadienyl sandwich compounds: synthesis, structure and chemical bonding (Chem. Commun. - <https://doi.org/10.1039/C9CC09018E>) - Work performed by the Layfield group (University of Sussex) produced two novel uranium half sandwich complexes. Attempts to produce a sandwich complex, $[U(\eta^4-C_4R_4)]$, led to ligand activation by deprotonation of a trimethylsilyl substituent, which has significant implications in the field of small molecule activation. The NCS produced the diffraction data for one of the two novel half-sandwich complexes, as the crystals produced were not good enough quality to be run using their in-house diffractometer.

Advanced Techniques Highlights

The advanced techniques provided by the NCS perform solid-state chemistry studies and drive a range of transformative research areas. They centre around the use of in-situ diffraction experiments to monitor in-operando dynamic processes in complex systems, which addresses major global issues as well as providing fundamental understanding e.g. providing atomic resolution detail as to how MOFs can be utilised for carbon capture and hydrogen storage while variable temperature work sheds light on the functioning of organic electronics and catalysts. The techniques provided are variable temperature, high pressure, gas cell, charge density and access to neutron single crystal diffraction.

During the reporting period a number of exciting results were published across these techniques, some notable examples including a variable temperature study (Gass, Univ. Of Brighton) revealing a spin-crossover transition (<https://doi.org/10.1039/C9DT03412A>), a neutron study (<https://doi.org/10.1002/chem.202000016>) revealing a critical Gold Hydride transfer mechanism and a charge density study (DOI: [10.1016/j.molstruc.2020.129270](https://doi.org/10.1016/j.molstruc.2020.129270)) that presented a novel approach to elucidating structure-property relationships in pharmaceutical co-crystals. The NCS development and application of an in-situ gas cell has been a particularly active area of research with the case study associated with this report presenting a particularly successful collaboration with Prof Weller (York) which is concerned with the generation of “impossible” complexes and catalysis in single crystals. This work has seen a number of publications, with the most recent (DOI: <https://doi.org/10.1002/anie.201914940>) reporting a novel sigma-alkane Cobalt complex generated by in-situ single crystal hydrogenation in the very high impact factor journal *Angewandte Chemie*.

Methods Development

NCS signed a 3-way contract with the global chemical company Merck and instrument manufacturer Rigaku to run a Joint Evaluation Project on the “crystal sponge” method. This project aims to provide a new service to both the academic and industrial sectors to obtain structures of uncrystallisable materials or compounds that can only be produced in exceptionally small quantities. Rigaku supplied NCS with a new state-of-the-art diffractometer exclusively to conduct the work and Merck are providing the sponge materials and extensive training. An EPSRC Impact Acceleration Account project was also funded in parallel to establish a dedicated facility and project manager and explore the service provision model, begin community engagement and develop commercialisation potential. Training visits were made by Rigaku and to Merck. Despite the pandemic restrictions, the diffractometer has been installed and a dedicated sponge soaking laboratory established. Benchmarking reproducibility studies have been successfully conducted and novel results are now being generated. Two PhD studentships have been secured and will

contribute to the scientific developments in the coming reporting period, as well as building commercialisation opportunities with Merck.

The NCS has pioneered work to increase understanding of radiation induced decay in small molecule single crystal samples and develop mitigating data collection strategies. In collaboration with macromolecular crystallographers (Garman, Oxford) our publication (<https://doi.org/10.1107/S2052252519006948>) is the first report of this effect in small molecule crystallography and illustrates its seriousness, breadth and impact to the entire community. This has triggered an international collaboration (Dr Grabowsky, Bern) to establish a standard approach at synchrotron radiation sources which has begun with beamtime at the Advanced Photon Source (Chicago, USA) and time awarded at the ESRF Swiss-Norwegian beamline (postponed due to Pandemic restrictions). This work will also have a significant impact on emergent areas which suffer from this effect such as the Crystal Sponge technique and Micro Electron Diffraction and the NCS is planning work with Rigaku in this area.

Community Leadership

During this period a significant review in the journal/book hybrid 'Structure & Bonding' was spearheaded and written by Simon Coles. The review is entitled 'Leading Edge Chemical Crystallography Service Provision and Its Impact on Crystallographic Data Science in the Twenty-First Century'. It describes the equipment, infrastructure and processes required to operate such a cutting edge and large facility, bringing in synchrotron radiation developments. It then describes how such facilities feed into databases, in turn fueling a range of different data mining and other research activities, and is beginning to enable data science in the chemistry-based disciplines. This review also contains extensive supplementary material comparing facilities data and when the book is published in early 2021 it will become the formal citation for the use of the NCS.

The Director is a member of the International Union of Crystallography's Committee on Data (CommDat) and is heading up a global community consultation on the curation, use and reuse of raw data in chemical crystallography. This work will inform policy at IUCr which will be cascaded out to all national bodies and journal publishers. An article in the IUCr Newsletter by Simon Coles (<https://www.iucr.org/news/newsletter/volume-28/number-1/raw-data-availability-the-small-molecule-crystallography-perspective>) reports the results of engaging the global community and is the foundation of a workshop organised by him at the IUCr Congress and General Assembly (postponed from Aug 2020 to Aug 2021).

Simon Coles is the Chemistry lead for GO FAIR, an EU initiative aimed at making research data open. This work has led to a significant involvement in driving this agenda forward with the International Union of Pure and Applied Chemistry and Simon is a member of the IUPAC Task Force on FAIR data which will report its recommendations for implementation in 2021.

Publications

The number of publications that the NCS is associated with is very considerable a three-year list is too long to incorporate into the body of this report and so is appended at the end. The NCS generates different types of outputs that are dictated by the type of operation – these are crystal structure characterisations where NCS collects data and passes it to a user to work up, analyse and report; crystal structure determinations that NCS performs and reports in collaboration with users; larger scale projects where NCS drives the research and its publication.

Crystal structures invariably form a key component of a paper if it is possible to acquire them – for many they are an invaluable, definitive characterisation of a new chemical compound and therefore are always considered critical to a paper. We therefore choose to categorise the papers in the following way (indicating how they might be equated to H, M, L as requested, however we stress that this is inappropriate for NCS operation).

The NCS publication categories are thus:

- **DCO** (Data Collection Only – approximately equivalent to L). NCS collects data on samples which cannot be examined using local facilities or where there are no local facilities - the user solves, analyses and publishes the data themselves. The user is required to at least acknowledge the service in the publication using a particular form of words and preferably also cite a paper outlining the NCS operation (Coles & Gale, *Chem Sci*, 2012, 3, 683-689). Publications are therefore tracked in several ways – searching for the acknowledgement, sifting citations of the NCS paper and requesting returning users to provide publication outputs. Tracking of these papers can at times be difficult to enforce and accurately perform – we believe there are likely to be some additional papers however it is not a sensible use of staff time to take the additional measures required to trace these.
- **FSA** (Full Structure Analysis - approximately equivalent to M). NCS collects, solves and analyses data on samples which cannot be examined using local facilities or where there are no local facilities – NCS collaboratively publishes the crystallography results in a publication driven by the user. NCS staff are authors on the publication, which facilitates tracking (supplemented with searching for the acknowledgement, sifting citations of the NCS paper and requesting returning users to provide publication outputs).
- **C** (Crystallography led study - approximately equivalent to H). A study led by the NCS or where the facility has played a core role. These are solid-state structural chemistry studies as opposed to those performing crystallography for the purpose of characterisation of a new compound. These papers are often based on the NCS advanced techniques and methods development and would not be possible without NCS staff expertise and state-of-the-art instrumentation. NCS staff are always co-authors, enabling accurate tracking.

For the 2017-20 outputs we report a total of 204 publications (although there are some DCO that are likely missing and some 2020 papers yet to be indexed by the citation services). The 2012 perspective article containing details of the NCS operation (Coles & Gale, *Chem Sci*, 2012, 3, 683-689) outlined the NCS operation. This ‘highly cited paper’ continues to be in the top 1% based on Web of Science’s highly cited threshold for the publication year and field.

Impact

Training courses and workshops.

Several of our usual workshops and training activities were scheduled (‘Introduction to Crystallography’, ‘Approaches to Modelling Disorder’ and 1:1 work shadowing/training) but all had to be postponed either due to UCU strike action or restrictions imposed by the COVID-19 pandemic.

Activities to promote the facility beyond its core user base.

This period included a significant Community Statement of Need exercise, which reached far beyond the current user base and explored numerous new areas for activity and support – the process and

outcomes of this are detailed in the User Survey section below. Numerous planned events, such as conference sponsorship and seminar presentations (eg Lincoln and Nottingham Trent Universities), were postponed or cancelled due to the pandemic lockdown situation. The coordination chemistry community was engaged through sponsorship of the RSC Dalton Southern Region meeting in Oxford on September 18th 2019. The NCS was included in event branding and the Director attended, distributed promotional materials, addressed the conference and coordinated the poster judging (which involved engaging with all poster presenters).

In the last annual report we detailed a Physics Today article about the solution of a 120 year old problem which revealed a new chemical phenomenon – this was followed up by a full article this period distributed to 50,000 RSC members in Chemistry World, see <https://www.chemistryworld.com/news/solution-to-120-year-old-puzzle-reveals-new-chemical-phenomenon/3010955.article>. During this reporting period Simon Coles continued to be the interim/emergency editor of the British Crystallographic Association quarterly magazine, Crystallography News. In this role he promoted the NCS directly through pieces in the magazine and by building links with other national society magazine editors (Switzerland, Italy & USA) where he wrote short commentary pieces mentioning the NCS.

Public engagement.

Simon Coles led a major event at the University of Southampton campus to mark the International Year of the Periodic Table on 22nd November 2019. A 3-minute video about the sustainability of the elements was projected onto the Life Sciences building and an associated science fair, sponsored by the NCS with numerous crystallography activities, was held. This highly successful event was featured, including producing the lead image in a full article in Chemistry World, see <https://www.chemistryworld.com/rsc/celebrating-the-iypt-in-style/4010835.article>. Furthermore, Simon led a project involving the global crystallographic community where the periodic table is illustrated through crystal structures: entries for elements were authored by crystallographers young and old (<https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/contributors/>) and with news items each element released over the course of the year. This was in collaboration with CCDC and the outcome can be seen at:

<https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/>. This work is being continued through funding from the RSC to develop learning materials and activities for schools and the general public that are built on top of this resource.

Through the Scouts, Simon Coles organised a small local science fair, including a show on how “Crystallography reveals COVID-19”. This was to be a primer for the NCS annual SOTSEF science festival activity which was cancelled at the last minute due to nationwide lockdown. SOTSEF was held as an online event in May and the NCS participated by developing online digital material,

https://www.sotsef.co.uk/science_engineering_day/?zone=chemistry. The NCS took the opportunity to develop online public engagement materials and another lockdown project with CCDC developed “BattleCards”, a downloadable and printable variant of the popular Top Trumps game, linked to the Periodic Table built for the international year, see

<https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/activities/>. A summer student then went on to enable this game on the Instagram social media platform.

Facility staff training and career development.

Drs Bannister and McCormick joined the team as Service Coordinator and Scientist respectively – they undertook probation mentoring and a range of skills development courses including Invoicing; Budget holder training; Financial reports training; Radiation safety training refresher; Tutoring. While most scheduled conferences were postponed in this reporting period, there was a proliferation of online courses during the pandemic and so a mixture of face to face and online training was achieved. All team members partook in the extensive Rigaku crystallography school, which was in effect a week-long course. There were also numerous other online talks, webinars, conferences, workshops, courses and demonstrations attended by at least one member of the team e.g. Processing of a twinned data set in CrysAlisPro and structure solution in Olex2; Crystalline sponge method; High Pressure Data

Processing, 13th high pressure diffraction workshop. The most prominent in-person training activities were based round the Crystal Sponge project and involved a 1 week visit from a senior member of the Rigaku Tokyo team and a hands-on visit to Merck's laboratories in Darmstadt.

Cost Recovery

The NCS is free at the point of access, which is the only viable financial model. This is because a) researchers cannot predict in advance whether they will produce samples that could only be investigated using advanced facilities/expertise and b) only some samples for a particular study will require advanced facilities whilst the remainder can be studied locally. For such a mixed model it is impractical to implement and anticipate anything other than a 'free-at-point-of-access' mechanism. Also access to synchrotron facilities is already free at the point of access and therefore charging to access via a NCS is incompatible with this model. Access to the NCS is subject to peer review on scientific merit and moderated to ensure the volume request is appropriate for the project being supported, which prevents access purely to avoid paying local charges.

However, some cost recovery is obtainable through a very successful commercial service. The commercial arm of the NCS serves the pharmaceutical industry with a professional and efficient service – it is used by a number of different companies, including big pharma. Additionally, it is possible to recover some costs from external grant applications – up until now this route has been somewhat limited and has tended to cover capital more than running costs.

| Year | Running Costs | Grants | Other Academic | Students | Industry | Other | % |
|------|---------------|--------|----------------|----------|----------|----------|------|
| 2017 | £602,000 | | | | £18,000 | | 2.9 |
| 2018 | £576,000 | | | | £35,000 | | 6.1 |
| 2019 | £514,000 | | | | £49,000 | | 9.5 |
| 2020 | £465,000 | | | | £36,000 | £12,000* | 10.3 |

Costs rounded to the nearest £1000

*Staff costs awarded in the EPSRC Impact Acceleration Account grant.

Figures reported are for the calendar year (Jan-Dec). The commercial service has expanded year on year since its establishment in 2017. Considerably more business was anticipated in 2020, but this was significantly limited due to the shutdown and cautious reopening caused by the COVID-19 pandemic lockdown (March – August). The pandemic did result in reduced running costs and therefore this coupled with the IAA grant income resulted in the cost recovery target of 10% for the period being exceeded.

There is potential for more cost recovery if different activities are embarked on and the Statement of Need exercise identified a number that would result in cost recovery. These form the basis of our future plans.

- A significant increase in advanced techniques work was clearly considered worthwhile and would be in demand. We anticipate this initially being free at the point of access in order to perform proof of concept work. Proof of concept would be expected to lead to incorporation (and therefore funding) into larger, funded project proposals e.g. to research councils and charities.
- Additionally, a crystallisation service was considered a very worthwhile addition. This would lend itself both to external grant income and to a highly attractive commercial service. We expect to incorporate our Crystal Sponge service into this endeavour, as well as other innovative crystallisation technology.

Users

NCS users fall into six categories:

- a. Research Group Principal Investigators. We do not record the number of students for each PI accessing the NCS, however an accepted estimation an average user would have 2-3 students (although some groups are well into double figures).
- b. UK service crystallographers. As 'gateway' users, this access mode supports large numbers of researchers, as departmental crystallographers access the NCS to analyse difficult samples from across *their* entire user base.
- c. Collaborators using Advanced Techniques.
- d. Commercial Users. All of these are from the health and pharmaceutical sector.
- e. International Collaborations. More details are provided in the Links section of this report.
- f. People accessing the training programme. There were no face-to-face training activities held in this period (see Impact section of this report).

Prospective academic users (categories a-c above) must make an application in response to a six-monthly call to access the NCS. This application must estimate an allocation of expected samples that will require the NCS facilities i.e., there is great uncertainty as to how many new compounds will be made, how many of these can be crystallised and how many of these will be of lesser quality and therefore not examinable with local facilities. Furthermore, departmental service crystallographers (category b above) apply on behalf of several academics in their department, further increasing the uncertainty around the likely number of samples that will be produced. On application these users are asked to identify academics they are submitting on behalf of, however no information on numbers of students, PhD candidates or PDRAs is requested from category a-c users due to the significant additional requirements that would be placed on users to gather this information for an application relating to speculative samples. We cannot therefore report on the level of granularity of users as requested. It should also be noted that commercial users are counted as companies, not individuals, and within each company there are generally many research scientists who use our services but through a gateway user - again we do not request this level of information of our clients.

Furthermore, the NCS has not previously kept records of new and repeat users, but this information is now included here for the first time. The user information presented in the table below is therefore that which is most appropriate for the NCS and which we are currently able to gather.

| Year | Academic | Industry | Other | No. Repeat | No. unique |
|------|-----------|----------|-------|---|---|
| 2017 | 62 | 3 | 42 | | |
| 2018 | 65 | 8 | 49 | | |
| 2019 | 66 | 6 | 51 | | |
| 2020 | 67 (+48)* | 7 | 0** | 6 repeat industrial, 56 repeat academic | 1 new industry contact, 11 new academic |

* There were 67 unique users with an active allocation. Of these, 9 are service crystallographers (in other departments) and this enables gateway access for 48 further academic research groups.

** Due to pandemic restrictions none of the usual training programs were run this year, which would have accounted for 'other' users.

Research Areas

NCS users originate from 40 different institutions. Approximately 85% of our users are based in chemistry departments, while the remaining 15% originate from chemical engineering, natural science, materials science, defence materials, pharmacy and biochemistry departments. The geographic spread of users is even and touches all regions of the UK. User groups cover 23 EPSRC Research Areas with a further 3 categorising themselves as 'other' - this represents an increase of two areas on the previous 2018-19 report. The most common research areas include catalysis, chemical structure, synthetic chemistry (organic, supramolecular, organometallic, inorganic etc.), carbon capture, energy storage, small molecule activation, materials for energy applications.

User Surveys / Satisfaction

Users are generally satisfied with our service and we get a steady stream of praise through day-to-day interaction such as emails and telephone conversations. Some unprompted quotes that have been sent throughout the reporting period follow:

"Particularly in dealing with difficult crystals, you have contributed a great deal to our ongoing research. Without your valuable work we would not have achieved what we, and our Collaborators, have in our research" - J. N. Low, University of Dundee

"Thank you very much for all your efforts and contributions to help our project to answer a very important question with fast turnaround. Very highly appreciated!!!" - A. Pettersen, Astra Zeneca

"We have had a good collaboration over the years and I am extremely thankful. Smaller Chemistry Schools/Depts would not be able to function without the NCS service." - M. Beckett, Bangor University

Under normal circumstances we would have had user satisfaction comments relating to NCS training events, however as noted elsewhere, there weren't any run in this period. We have however found that maintaining and supporting education and PhD student training during the pandemic is crucial and we will be developing this further. We include some feedback on one specific education support activity that was conducted:

"I just wanted to say thanks to all of you for the great job you did in getting all the samples that I sent down to you over the last couple of months collected and the data back to me in time to work up for this year's cohort of final year students, it was a big ask and I know that you are always busy. Every student that submitted samples got at least one structure for their reports and a couple have more than five each, which is an unprecedented outcome for our projects and I think this has really shown the value of the technique to the wider department, so I'm hopeful of even more uptake next year." - G. Miller, Manchester Metropolitan University

Due to the requirement for a community driven Statement of Need exercise (SoN) to be conducted during this period, there had been significant engagement and various mechanisms for feedback and input – both from current and potential users. Concerned that we would cause a level of 'survey fatigue' which would not provide meaningful feedback, it was decided not to conduct the usual satisfaction survey at the same time.

For more information on the results of the community driven survey a link to the full Statement of Need and also to a summary of the results is provided below.

Link to Survey Results - <http://www.ncs.ac.uk/files/EPSRC-statement-of-need.pdf>

Link to Statement of Need – http://www.ncs.ac.uk/files/Statement_of_Need_2020.pdf

Alongside the positive feedback we usually receive, shown above, via email and telephone communications, the SoN exercise demonstrated considerable appreciation for the current service and some comments provided include:

"The NCS is an outstanding service of very great value to the chemical community in the UK!" - P. Knipe, Queens University Belfast

"The national crystallographic facility provides an essential research capability for research groups who do not have access to local instrumentation. The national facility is an efficient, economic and sustainable approach to meeting the requirement for the collection and interpretation of crystallographic data which is the cornerstone of much chemical science." - N. Bricklebank, Sheffield Hallam University

"While we have an ancient, unreliable diffractometer in our home laboratory, we can, at best, obtain publishable data from about half of the samples submitted. The 'difficult' half get sent to the NCS where the staff and state of the art instruments work wonders and provide good results for many of the samples we send. In times of local instrument breakdown all samples are sent to the NCS and the work of our synthetic chemistry groups would grind to a halt without them. NCS's ability to deal with weak diffractors and twinned crystals is really essential for our work." - M. Elsegood, Loughborough University

"The NCS was invaluable during an extended period when our home facility was very unreliable." ... "The expertise is also invaluable - there are one or two samples (including datasets acquired at home) where we simply would not have got a result without their help." - J. Fielden, University of East Anglia

"This is a fantastic service that is essential for many researchers in universities where there is no single crystal diffraction facility. Without it we could not carry out our research." - G. Hogarth – Kings College London

Whilst it was decided our annual user survey would not run this reporting period, typically it would normally be circulated to active users at the same time as the biannual call for applications to access the NCS. This would request feedback on the following:

- The NCS ease of use, e.g. ease of application, clear sample forms and guidance
- The NCS responsiveness to user requests, e.g. rapid turnaround, additional data collections
- The NCS as helpful with regard to publication, e.g. all data necessary provided, assistance with crystallography sections etc. as per type of service requested
- Whether the user would recommend the NCS to a colleague
- Any further comments

The annual user satisfaction survey will be resumed in the next reporting period.

Service Demand

The service provided can be separated into two types based on the extent of the study (see also Publications Section) - Full Structure Analysis (FSA) and Data Collection Only (DCO). The DCO service is for experienced users requiring access to more advanced instrumentation at the NCS. The FSA service is accessed by users who are not familiar with solving crystal structures or require the help of expert crystallographers for particularly difficult structures. The fundamental difference is that the DCO service essentially only requires instrument time and is relatively quick to turn around (although this is not always the case). The FSA service requires the same amount of

instrument time but a considerable amount of expert crystallographer input to generate a result. The Service Level for processing the data resulting from the DCO service is 5 days, whereas the target for processing FSA samples is 20 days.

On application, an allocation is awarded which is prioritised into high, medium and low priority samples. On receipt a sample is logged into our Portal system with time until data collection Service Levels of 10, 20 and 30 days for High, Medium and Low priority samples respectively (this prioritisation system is regardless of whether a sample is FSA or DCO as prioritisation is based on scientific merit).

All commercial samples are FSA, but instead of L/M/H priority these are treated as bands 1/2/3. This banding refers to the difficulty of the sample and therefore how much resource is likely to be required to generate a result. The banding is directly linked to a pricing structure. Band 1 requires less than 4 hours on an instrument and is a relatively simple structure to solve; Band 2 is between 4 and 24 hours on the instrument and is reasonably difficult to process; Band 3 includes any sample requiring > than 24 hours data collection or a particularly challenging data analysis. Whilst these figures don't specifically align to the high, medium and low brackets for academics, they provide an indication of instrument time required for routine, difficult and extremely challenging samples. It is noted that processing times can vary drastically depending on sample difficulty. The table below summarises the Service Level criteria for DCO and FSA analyses.

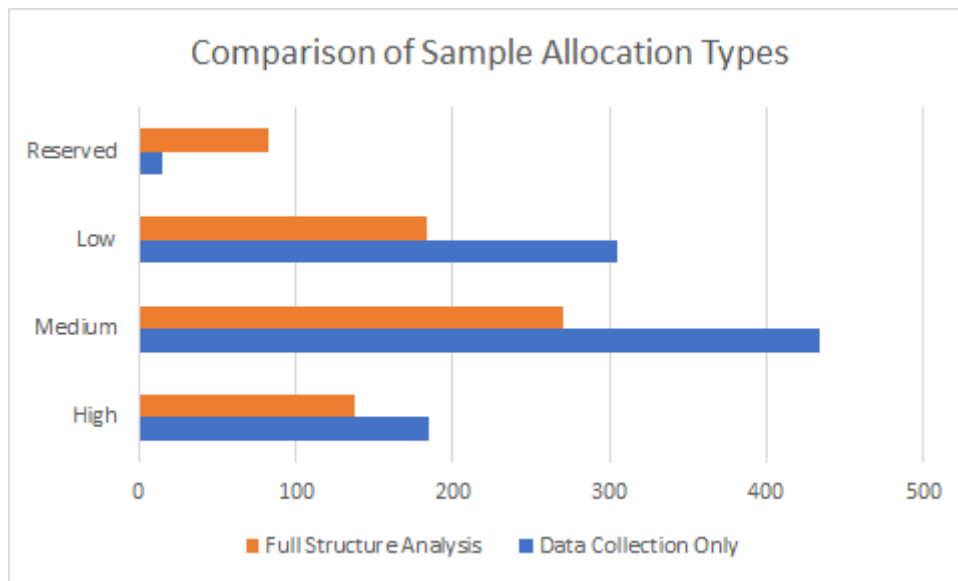
| Service | | | Commercial | |
|---------|------|------|------------|--------|
| | DCO* | FSA* | Band | Time** |
| H | 15 | 30 | 3 | >24 |
| M | 25 | 40 | 2 | 4-24 |
| L | 35 | 50 | 1 | <4 |

* Total number of working days to provide result

** Time on instrument (hours)

Theoretical Demand

The NCS operates a biannual call for applications for access allocations. Academics apply for the number of samples they expect their group will generate in a 6-month period. The NCS Strategy and Allocations Panel (SAP) review this request on scientific merit and to ensure a reasonable workload for the service. An additional category, 'Reserved', is introduced at this point: if a large request is made then some samples can be allocated here – these will not be included in Service Level reporting and are examined only if there is spare capacity and no turnaround time guarantee is given. The Reserved mechanism allows the service capacity to be fine-tuned at the stage when the demand is essentially unknown. This is the basis of *theoretical* demand and capacity levels. The number of samples allocated during this reporting period are shown below.



The ratio of H:M:L is allocated to provide an appropriate workload. While there is a higher proportion of DCO samples, over 40% of the capacity relates to FSA samples, which are more demanding of time and expertise.

Actual Demand vs Capacity

Having defined the capacity for samples that could theoretically be submitted, it is now possible to match this to actual demand in the reporting period. The average number of days between a logging in a sample and it being examined on an instrument is tabulated below.

| | | Number of days for sample to progress | | Overdue Samples | |
|---------------|-------|---------------------------------------|----------------|-----------------|---------|
| | Count | Mean | Threshold Days | Count | Percent |
| Total | 402 | 13.9 | | 40 | 10.0% |
| Low | 110 | 24.5 | 30 | 15 | 13.6% |
| Medium | 158 | 13.1 | 20 | 9 | 5.7% |
| High | 134 | 6.0 | 10 | 16 | 11.9% |

This shows that 90% of samples were run on the instrument within the threshold time. Given the complications throughout the year due to COVID-19 restrictions, this is indicative that this aspect of operation matches demand from users. The number of days between a sample being run and the data being processed is summarised below.

| | | Number of days for sample to progress | Overdue Samples | | |
|--------------------------------|-------|---------------------------------------|-----------------|-------|---------|
| | Count | Mean | Threshold Days | Count | Percent |
| Total | 434 | 13.3 | | 78 | 18.0% |
| Full Structure Analysis | 153 | 26.4 | 20 | 30 | 19.6% |
| Data Collection Only | 281 | 6.1 | 5 | 48 | 17.1% |

In this respect it has been harder for capacity to meet demand. Processing data can be a very time consuming and complicated process. Whilst the number of DCO samples submitted is a higher percentage than those expected, over 1/3 samples (35.2%) are for the FSA service.

The purpose of the NCS is to examine particularly complex and challenging samples that cannot be address by users' local facilities. In the current period of funding the NCS has made significant improvements to its equipment base - particularly with a new generation of detectors, maintaining it as one of the most powerful facilities in the world. This in-turn has resulted in a much more rapid generation and acquisition of data – not only faster, but on even more demanding samples. Accordingly, we are now experiencing a more serious bottleneck at the data processing stage, due to the greater demand on expert staff time.

Theoretical demand this year was much higher than actual demand as for large parts of the year the country was in lockdown and to alleviate some pressures on groups allocations were rolled over from Sept to May to minimize administrative demands on our userbase.

Risks

A risk register is maintained for all capital equipment, either whole entities or components where appropriate, that the facility crucially relies on and has a value >£10k. The register is regularly reviewed by the Operations and Management Team (OMT), which passes concerns or strategic requirements to the Strategy and Allocations Panel (SAP).

In this period an opportunity to bid for Core Equipment arose and the register readily identified a goniometer and a cryostat as requiring replacement (the former had been returned to the factory for a persistent critical problem that couldn't be resolved in the field, while the latter had been in service for nearly 20 years and in imminent danger of complete failure). The register also identified a persistent water chiller problem causing failure of the most important X-ray generator in very hot weather – a replacement is being procured.

Other facility related risks are assessed by the OMT and/or SAP as appropriate. NCS is embedded in School of Chemistry strategy, with the Head of Department attending OMT once a quarter and SAP twice a year, which ensures senior management are aware of major issues. The risks considered include:

- Those associated with staffing absence or resignation - reasonable number of PDRAs so some redundancy, Director covered by department,
- Financial - regular review to ensure overspend, contingency plans if funding renewal doesn't occur,
- Disaster recovery e.g. fire, pandemic – covered by Departmental policy and mitigation/recovery measures put in place,

- Host institution issues e.g. infrastructure failure – reporting channels clear, close two-way interaction with School Facilities Manager.

Management of the current Covid-19 pandemic situation illustrates the strong risk prevention measures in place. The department cautiously opened soon after the first lockdown ended in June 2020, with the NCS amongst the first to return due to the low level of laboratory occupancy required and high potential for remote control and monitoring of experiments. Prior to return, extensive and rigorous Risk Assessments and Method Statements were devised at several different levels – research groups leaders were engaged and trained from the outset and templates cascaded down through the levels to ensure risk levels minimised. Controlled access and occupation levels were devised and coupled with rigorous hygiene and PPE measures to ensure infection control. Weekly reviews were performed and reported up the chain of command. With time the department moved to different tiers of control which involved gradual increase of occupancy with associated review and rewrite of RAMS processes and documentation. Extensive Covid-19 safety training has been provided to all staff reoccupying the buildings with documentation, meetings and support provided via online systems. A rigorous system of notification, risk assessment and sign off is required when further staff, servicing engineers, etc are admitted into the department. Throughout this time a dedicated member of senior staff has overseen the Covid-19 response and risk assessment. The NCS has been deemed business critical, with suitable procedures in place, meaning that it will be amongst the last operations to be shut down in the case of further lockdown.

KPIs and SLs

| Type | Description | Time for Performance | SLA Level | | | 1st Sep 2019 - 31st Aug 2020 | Directors Comments |
|------|---|--|-----------|-------|-----|--|--|
| | | | Green | Amber | Red | | |
| RMI | Total number of all Users | Period associated with specific report | N/A | N/A | N/A | 67 Routine Service users (+48 users via departmental service crystallographers) | No training activities conducted this year |
| RMI | Spectrum of user types | Period associated with specific report | N/A | N/A | N/A | 59 Individual service users 8 Departmental Crystallographers 8 Commercial clients 7 Advanced techniques | |
| RMI | Number of University / Research Groups Involved | Period associated with specific report | N/A | N/A | N/A | 40 Institutions / 94 Groups | |
| RMI | Percentage of Access Requests Accepted | Period associated with specific report | N/A | N/A | N/A | 100% (Routine service) / 100% (Advanced Technique) | |

| | | | | | | | |
|------------|--|--|---------------|---------------|-------------|---|---|
| RMI | Percentage of equipment time dedicated to different access modes | Period associated with specific report | N/A | N/A | N/A | 60% (Routine service, academic) / 10% Commercial / 20% Host institution / 10% (Advanced techniques) | |
| RMI | The number of data sets processed | | N/A | N/A | N/A | 535 | Until mid-March were on target for a 'normal' year - COVID restrictions caused a significant drop in submissions from then. |
| SL | Percentage of User enquiries responded to within Stated Window | 2 working days | 95% and above | >90% but <95% | 90% or less | 100% | |
| SL | Percentage of Access Requests Responded to within Stated Window | 2 working days | 95% and above | >90% but <95% | 90% or less | 100% | |
| SL | Percentage of Training Requests Responded to within Stated Window | 2 working days | 95% and above | >90% but <95% | 90% or less | 100% | |
| SL | Percentage of Training Requests Delivered within 3 months | 3 months | 95% and above | >90% but <95% | 90% or less | 100% | |
| SL | Number of Customer Complaints (expressed as a percentage of the Total Number of User Approvals made within the period) | Period associated with specific report | Less than 5% | 5-10% | Over 10% | 0% | |

| | | | | | | | |
|----|--|--|---------------|---------------|-------------|-------|-------------------|
| SL | Percentage of customer complaints resolved within Stated Window using the Dispute Resolution Plan. | Period associated with specific report | 95% and above | >90% but <95% | 90% or less | n/a | |
| SL | Percentage Uptime /Downtime of Total Available Time within Period | Period associated with specific report | 95% and above | >90% but <95% | 90% or less | 100% | See Note 1 below. |
| SL | Percentage of Access Costs recovered | Period associated with specific report | 10 | 6 | 2 | 8.7% | See Note 2 below. |
| SL | Number of Publications | 1 year | 30 | 20 | 10 | 50 | |
| SL | Number of publicity activities per year | 1 year | 10 | 8 | 6 | 10 | |
| SL | The time from arrival of a sample to logging in and informing a User of receipt | within 2 working days | 95% and above | >90% but <95% | 90% or less | 100% | |
| SL | The time a sample is in the queue | From logging in a sample to examination: High Priority sample = 10 working days | 95% and above | >90% but <95% | 90% or less | 88.1% | See Note 3 below. |
| SL | The time a sample is in the queue | From logging in a sample to examination: Medium Priority samples = 20 working days | 95% and above | >90% but <95% | 90% or less | 94.3% | See Note 3 below. |
| SL | The time a sample is in the queue | From logging in a sample to examination | 95% and above | >90% but <95% | 90% or less | 86.4% | See Note 3 below. |

| | | | | | | | |
|----|-------------------------------------|--|---------------|---------------|-------------|-------|-------------------|
| | | Low Priority samples = 30 working days | | | | | |
| SL | Time from examination to end result | Data collection = 5 working days | 95% and above | >90% but <95% | 90% or less | 82.9% | See Note 3 below. |
| SL | Time from examination to end result | Full Structure Analysis= 20 working days | 95% and above | >90% but <95% | 90% or less | 80.4% | See Note 3 below. |

Notes:

1. The impact of COVID-19 was extreme, however the NCS facility is considered business critical to the department and so was opened at the earliest possible opportunity after lockdown. Lockdown days are formally university closed days and so do not count towards this metric and accordingly the facility was usable 100% of the available time.
2. The revenue generated by the commercial arm of the NCS is increasing year on year. The COVID-19 pandemic lockdown reduced the amount of time available to perform commercial work considerably, but if extrapolated this increasing trend is still true for 2020. Further income was generated by including 50% staff time buy-out for the Crystal Sponge project via the Impact Acceleration Account award – however this only took effect in the last month of the reporting period and will be reflected in full in the next report.
3. All these Service Level metrics relating to turnaround time were affected by the COVID-19 pandemic restrictions on access to the workplace. The department was closed at short notice from mid-March to beginning of July, affecting samples already in the system. Restart was cautious and involved just one person accessing the facility to perform experimental work and this continued throughout July and August, thus also affecting performance. It should also be noted that commercial samples are now logged in the same system, yet they have different turnaround targets, thus skewing the metrics – we are investigating approaches to separating these.

Links

NCS has input and collaboration with numerous **Organisations and Facilities:**

- Diamond, through beamline I19 (EH1) are formally key partners in delivering the NCS. This has led to access and use of I19 EH2 and more recently to I15. Furthermore, Diamond and Southampton co-fund and supervise a PhD student aligned to the NCS and split over the two sites, whose goal is to develop and apply a new type of gas cell for in-situ/in-operando studies.
- A collaboration with the SXD beamline at the ISIS neutron source has seen the facilitation of access and data analysis for NCS users that wouldn't otherwise have been aware / capable of using such a facility. This has resulted in publications and a formal arrangement would be proposed for future delivery of the NCS.
- SJC is also the Director of the Physical Sciences Data-science Service and is driving convergence of the two NRFs on crystallographic data management, aggregation and publication.
- SJC advised on the models and approaches for establishing the Computed Tomography NRF and sits on management advisory panel of the Southampton site.
- SJC is a consultant feeding into the direction and setup for the ChemMatCARS beamline at the Advanced Photon Source (Chicago).
- Quantum Crystallography – consortium involving 20 parties across Europe aiming to embed this new approach into crystallography practice, mainly through training networks (SJC is a lead).

- Radiation Decay project through a collaboration with Dr Grabowsky (Bern) that is informing synchrotrons (specifically Diamond, APS and ESRF) as to how to deal with this phenomenon.
- BCA Education & Outreach Officer and CCDC – SJC coordinates public engagement initiatives and projects at a national level.
- SJC sits on the IUCr Committee on Data and IUPAC FAIR data taskforce – and through these Unions is driving global approaches to managing, curating and sharing raw data in Chemical Crystallography.

The following **International** institutions have formal links with the NCS, generally relating to student exchange and training and mostly resulting in collaborative papers:

- Karlsruhe Institute of Technology - PhD student placement and training, Nature paper published
- Radboud University (Nijmegen) – combined techniques to solve phase transition problems, several papers and student exchange
- King Saud University – collaboration leading to publications
- Wakayama University – student visits and several papers using the charge density technique
- University of Malaya - student training visit and papers published
- University of Mauritius - SJC conducted a training workshop, leading to several papers
- University of Ghana and KNUST - SJC held several training workshops under Royal Society and Leverhume projects, resulting in being a Local and Scientific Organiser of the PCCr2 Pan-african Conference on Crystallography in Accra. Application for World University Network funding for researcher mobility between Southampton and UoG in progress
- University of Cagliari – long collaboration (SJC visiting Prof providing training many visitors to NCS – 1 student in this reporting period, Enrico Podda via Erasmus scheme).
- Turkey (Zonguldak & Gebze – SJC visiting academic) continual stream of papers and visits (Gebze student Erasmus visit during reporting period).
- SJC is responsible for setting up and coordinating Cagliari and Gebze as Erasmus exchange partners with Southampton
- UCAD Senegal – Ibrahima Thiam training visit in the reporting period, 3 papers published
- Yaounde University (Cameroon) – SJC provided a training course, resulting in a stream of papers.

Improvements and Future Plans

An EPSRC Core Equipment proposal was planned and written during the reporting period. It was awarded with an uplift and the equipment is on order at the time of writing. This funding replaces ailing components as well as providing new capability. A new goniometer for the high flux Mo X-ray source will replace a component that was at the top of the risk register and had perennial faults resulting in return to the factory for several months. A liquid nitrogen cryostat will optimise use of a new instrument secured as part of the Crystal Sponge project (see below). An Intelligent Goniometer Head will crucially enable more accurate centring for the smallest of crystals and an upgrade to focussing optics will make the new Crystal Sponge diffractometer the most powerful Cu-based diffractometer for chemical crystallography in the UK.

The NCS has teamed up with colleagues in the Department of Chemistry at the University of Oxford on an EPSRC Strategic Equipment proposal. This is for a new very low temperature enabled diffractometer in Oxford, to which NCS will have 10% access time, and which will provide an extended low-end temperature range (to ca 30K) and provide new capability for all NCS users. The outcome of the application is unknown at the time of writing.

The NCS is also involved in an ERC Advanced Grant proposal with Professors Weller (York) and MacGregor (Heriot Watt). If successful, EUSMOM will support the development of new cells and procedures to study catalysis in a single crystal in-operando.

Work will soon begin on extending the data infrastructure supporting the NCS facility – initially this is to integrate the new diffractometer, but this will lead in the medium term to a complete redesign and implementation with considerable new functionality and integration opportunities.

During this reporting period the NCS has embarked on a major methods development activity – the Crystal Sponge project. The concept is that an analyte that is uncrystallisable by traditional methods or only produced in minute quantities can be soaked into a MOF and the combined crystal structure determined. The NCS has formally signed up to a Joint Evaluation Project with the instrument manufacturer Rigaku and the global chemical company Merck. The aim of this project is to establish this concept as a service to both industry and academia. Rigaku has provided the NCS with a state-of-the-art diffractometer (worth £400k) for the project, while Merck has developed an approach to industrially synthesising the MOF host and is providing these gratis to the NCS for the project. The NCS role is to explore the scope of the technique and its application to academic research. EPSRC Impact Acceleration Account funding has been secured and is contributing to the setup of a dedicated support laboratory and buying out the time of an NCS employee (Dr James Orton) to manage the project and then develop the community engagement. The NCS expects to be able to provide the Crystal Sponge as a service to academia and to enter into a business partnership with Merck to collaboratively support industry.

The community Statement of Need exercise was embarked on in this reporting period (see above) and has surveyed the community at length. A case has been made for a crystallisation service including, amongst several techniques and approaches, the Crystal Sponge. There is also a requirement to significantly ramp up the most important advanced techniques – currently the NCS can only perform limited numbers of pilot studies.

Website

Please include a link to your website. What plans do you have to develop this space and what web analytics data do you have from visits?

The NCS website is split into our home site (link below) and our Portal site. The home site is used for people seeking information about our services, equipment and contact information. It also hosts our reports.

NCS Home Website - www.ncs.ac.uk

The publicly visible NCS home website is beginning to show its age (10 years since first launch) and so we will be making substantial changes to it in the coming period. This will initially involve reviewing, updating and adding content, but then migrating to a modern platform which we can bring in-house and readily have control over functionality and all content. Currently we do not have access to any web analytics in terms of content downloads, unique visitors to our pages etc, although this will be possible in the future.

The Portal site is considerably more up to date and advanced, providing an exceptional amount of functionality and is the primary interface between the service and its allocated/registered users. It is not public facing, but rather allows users to apply for an allocation, track their current samples, obtain data, view their history and interact with the NCS staff. The Portal site also has a significant internal administration function enabling much of the operation of the facility, including:

- establishing and managing a call for allocations and the subsequent application and review process (assigning members of the SAP to review and recording responses),
- assigning allocations,
- logging in/out samples,
- providing a prioritised scheduling in the facility based on Service Level rules for H/M/L samples,
- seamlessly tracking samples through the service workflow,
- associating data with a particular sample/allocation,
- providing a complete history of usage.

This enables NCS with ready access to information about the number of current samples, what stage each of those samples are at, due dates for certain parts of the workflow to ensure samples progress in a timely fashion on a day-to-day basis. On a more holistic level, it provides data on how many users there are total, how many are currently active, where they are based, what their interests in research are etc. This data extends to samples, such as how many have been processed in a given period, how many are DCO or FSA, or high, medium or low priority and enables us to gauge how efficiently we are keeping up with demand. The Portal system is also set up with rules regarding the specific KPIs and SLs that were determined at the outset of the current funding period and can readily report on these (adding new statistics is however a significant task).

The Portal sample submission interface is particularly important. When users submit samples, they provide information such as their experiment code, any solvents used in the preparation of the sample, whether the samples have any associated hazards, sensitive to light or air or moisture etc. Any hazards associated with solvents are automatically generated. The Portal system then generates an online form that NCS can access, and the user can print to include with their sample when it is posted. Once the sample arrives it is logged in and the portal system can automatically track the samples progress on the instruments. There is a help guide on the portal website to assist users through both the application and sample submission processes.

We do have plans for developing Portal in the short-mid term. Alongside fixes and inclusion of new metrics the main function we will develop is the interface to data – currently results data only is uploaded. In the future we wish to provide an interface that allows the user to access raw data as well, to perform some management and curation of their data and also the potential to make it readily available in a FAIR way so that it can be formally linked to publications and theses.

Case Study

We provide one case study with this report: Using in situ Single-Crystal X-ray Diffraction to Make “Impossible” Complexes. It may be accessed at the following link:

http://www.ncs.ac.uk/files/Andrew_Weller_Case_Study.pdf

And may be summarised as:

A collaboration between Professor Andrew Weller of the University of York and the University of Southampton’s National Crystallography Service is driving forward research into solid-gas transformations with molecular single crystalline organometallic materials. The research collaboration is helping to solve a decades-old problem to design catalysts which take the most abundant of all chemicals on earth – the hydrocarbons – and turn them into molecules of value that can enter the chemical manufacturing chain and be used for different applications.

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