

Title of Case Study: Southampton's National Crystallography Service helping researchers tackle key societal challenges

Grant Reference Number or Facility Name: School of Chemistry, University of Glasgow accessing National Crystallography Service, University of Southampton

One sentence summary: The University of Glasgow's School of Chemistry are one of the most prolific users of Southampton's National Crystallography Service.

One paragraph Summary: Data collected by the National Crystallography Service (NCS), at the University of Southampton, is enabling researchers at the University of Glasgow to explore the answers to some of the key challenges facing our world today such as the capture and storage of CO₂

Key outputs in bullet points:

NCS data is enabling:

- academics to fully explore their research and get it to a high quality publishable level
- the translation of research into real-world applications
- the understanding of structural features required for the storage of alternative fuels such hydrogen and ammonia in porous materials
- the development of porous materials that could be used for CO₂ capture
- the understanding of magnetic behaviour in materials
- the synthesis and characterisation of new molecular magnetic and nanomagnetic materials

Main body text

Data from the National Crystallography Service (NCS), at the University of Southampton, is enabling researchers at the University of Glasgow to explore the answers to some of the key challenges facing our world today such as the capture and storage of CO₂ and alternative fuels.

The NCS is providing Glasgow's School of Chemistry with a vital service that is enabling academics to fully explore their research and get it published in high quality journals.

For the past two years Glasgow has been sending up to 100 samples a year to the NCS for analysis and without access to this essential service, funded by the EPSRC, its scientists would struggle to fully exploit the potential of their research.

Experimental Officer in X-ray Diffraction Dr Claire Wilson said: "We have a couple of diffractometers at Glasgow but for lots of our research we can't get large enough crystals to use our equipment. Having access to the more powerful equipment at NCS and to the synchrotron at Diamond Light Source (DLS), in Oxfordshire, is really important to us. Without it we wouldn't be able to take our research to its full potential and generate the information required to take our research to a publishable level."

"The equipment at Southampton is a big step up to what we have here and there is also the added benefit of having access to DLS. We could apply directly to DLS but we would probably only be able to access it once or twice a year, whereas through NCS we get our samples dealt with in a really timely way."

Glasgow's NCS allocation is used across the School of Chemistry but there are a couple of research groups that make use of its services on a more regular basis.

Early Career Researcher Dr Ross Forgan's research group is exploring the development of porous materials that could have a significant impact on a number of key challenges facing today's society.

As the materials are porous on the nanometre scale it means they could potentially be used to store things such as gas inside of them.

Ross said: “There is the possibility to use them for capturing carbon dioxide, or for storing alternative fuels such as hydrogen and ammonia. They are very good at storing these materials in very large quantities without having to compress them.

“They could also be used in the fields of sensing or for storing drug molecules to be released into the body.”

However, because these porous crystals are full of holes and disordered, they diffract poorly and therefore, it is difficult to gain useful information from them.

Ross said: “The NCS has been really useful for my research group because our crystals tend to be around 50 microns in size and they don’t diffract well. The equipment that is available to us in Southampton is sufficiently powerful enough for us to be able to generate high quality data and enable us to publish our research.”

“This data is allowing us to progress our research further, and to fully understand the structure of our materials. One of our latest publications involving NCS data revealed how our porous crystals changed their structure during a reaction and helped us characterise that structural change using crystallography. This was an unusual and difficult thing to be able to do and the only reason we were able to characterise these changes was because of the quality of the data we obtained from the NCS.”

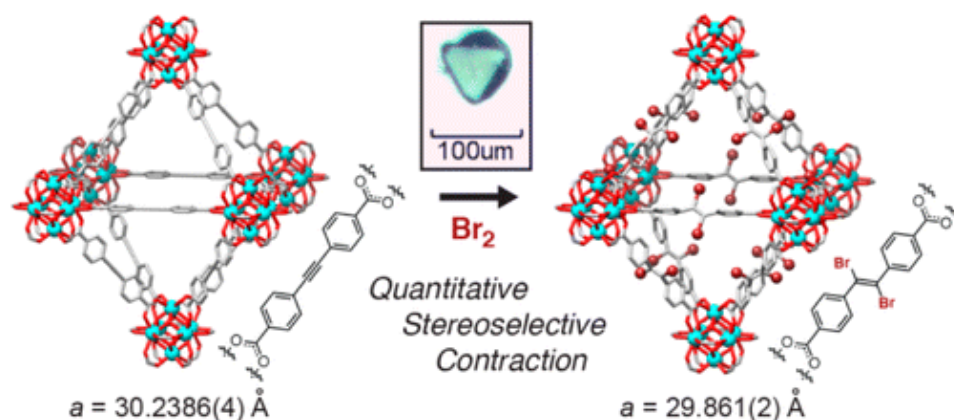


Fig 1. Crystal structures obtained from NCS data feature heavily in a recent publication from the Forgan Group *J. Am. Chem. Soc.* **2015**, 137,9527-9530

Another group that is a key user of the NCS is Dr Mark Murrie’s group that is exploring magnetic behaviour in materials, involving the synthesis and characterisation of new molecular magnetic and nanomagnetic materials.

The development of new synthetic strategies to assemble high-nuclearity transition metal complexes is a key target in modern coordination chemistry due to their fascinating magnetic properties.

Mark said: “Single-molecule magnet (SMM) properties give a tantalising glimpse of the possibility of the miniaturisation of information storage to the molecular level. SMMs are molecular, isolated as single-crystals and have a zero size distribution so that they can be used as tools to test magnetic theories and probe new magnetic phenomena at low temperatures in the quantum regime.”

However, the team’s research relies upon structural characterisation and due to the large size of the molecules and the weak diffraction of the crystals, they often require the data to be collected by the NCS.

Names of key academics and any collaborators: Claire Wilson, Ross Forgan & Mark Murrie

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