Diffraction

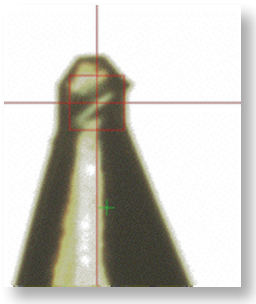
Small Molecule X-ray Crystallography

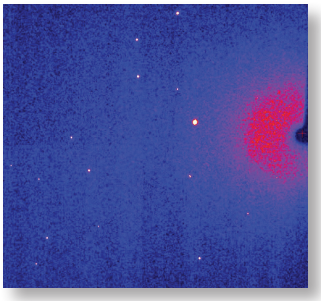
I19 Technical Information

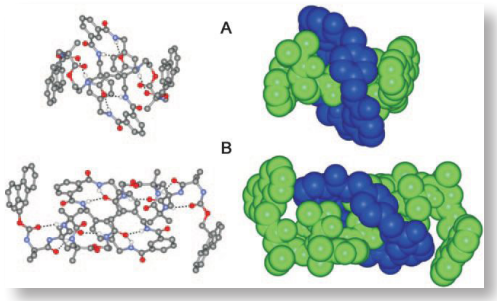
I19 - Small Molecule Crystallography

Small molecule crystallography is a well established technique for structure determination. However, even with advances in detector and laboratory source technology, there are still many cases where it is simply not possible to get a structure using conventional crystallography for a variety of reasons. This is where the power of synchrotrons can come to the aid of the crystallographer. By harnessing the extremely intense, focused X-rays, we are able to do experiments involving:

- small and/or weakly diffracting crystals;
- rapid collections on unstable samples;
- samples under differing environmental conditions;
- absolute structure and anomalous diffraction using the tuneable source;
- excited state studies.







Beamline Specification

	Experimental Hutch 1	Experimental Hutch 2
Diffractometer & detector	Fluid Film Devices 3-circle diffractometer with Dectris Pilatus 2M detector	Newport 4-circle diffractometer with Dectris Pilatus 300K detector
Energy Range [keV] / Wavelength Range [Å]	5 - 25 / 0.5 - 2	5 - 25 / 0.5 - 2
Temperature range	30 – 500 K	4 -1000 K
Typical beam size at sample (FWHM) [µm]	80 x 50 (H x V)	120 x 100 (H x V)
Other facilities	Facilities for handling air sensitive samples including Schlenk line and glove box, Diamond anvil cells for high pressure, X-Temp 2 crystal cooling device, gas rig for gas adsorption studies	

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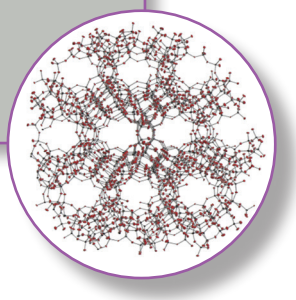
I19 Applications

Pharmaceuticals

- Accessing long wavelength X-rays allows determination of absolute structure of non-heavy atom molecules;
- Variable temperature and humidity experiments can be done to assess the stability of potential drug candidates;
- Structures can be determined which are intractable in the home laboratory thereby aiding regulatory filing.

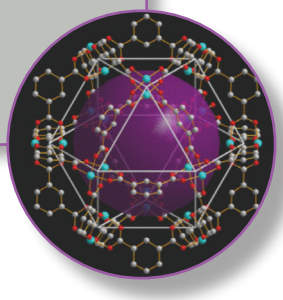
Chemicals

- The tuneable X-ray source allows the application of anomalous scattering methods to aid phasing;
- Catalysts can be studied under realistic environmental conditions using *in situ* gas cell;
- Structure determination for air sensitive samples is possible due to advanced crystal handling methods.



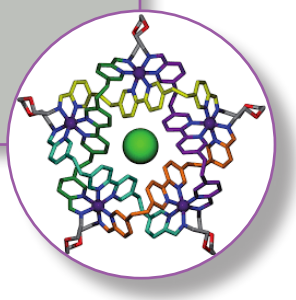
Functional Materials

- These materials are often produced as small, weakly scattering crystals which cannot be measured in the home lab;
- The extra intensity helps to locate light elements in heavy element frameworks.



Excited State Studies

- Laser excitation for study of metastable species;
- Pump-probe experiments using a chopper system – this allows for time resolved experiments for investigation of short-lived excited state species.



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