EPSRC D19 Single crystal & Fibre Diffractometer

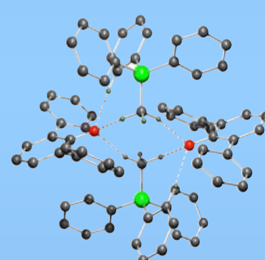
- D19 - a new diffractometer to be built in the next 12/18 months
- Funding from EPSRC (£1.2 million) and ILL
- Major new opportunities for experiments in crystallography & fibre diffraction
- The new instrument will produce a gain factor of 25 compared to the existing diffractometer
- Will open up new research areas in biology, chemistry, physics, materials and polymer science

J-F Clergeau of the ILL Detector Group shows the prototype D19 detector to Prof. Judith Howard, Univ. of Durham, while Alan Hewat, ILL Diffraction Group, looks on with satisfaction. *Right:* The new D19 diffractometer as visualised inside the instrument zone at the ILL

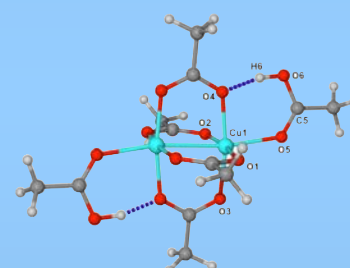
Crystallography

- Single crystal studies provide high resolution detail of the structure of chemical molecules
- Neutron crystallography provides unique information - for example, informtion on :
  - Weak intermolecular interactions
  - Fundamental studies of binding
  - Charge density analysis
  - Organometallic complexes and catalysis

Structural chemistry



Studies of the effect of strong intra- and inter- molecular hydrogen bonding on molecular geometry in carboxylate coordination complexes (Vives *et al*, 2001).

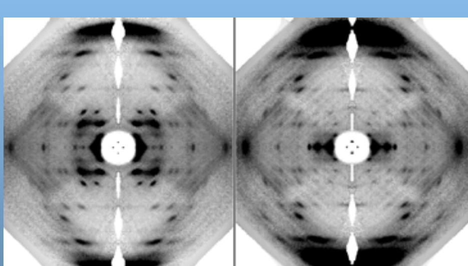


Hydrogen bonding in a phosphonium aryl oxide (Broder *et al*, 2002).

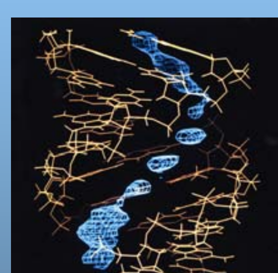
Fibre Diffraction

- Many important biological materials are fibrous in nature (eg nucleic acids, polysaccharides, filamentous viruses, amyloid)
- Many synthetic polymers have a fibrous texture (Kevlar, PET, PEEK, PEKK etc); this texture is important for their properties
- Fibre diffraction is the most appropriate method for the study of these filamentous systems
- Neutron fibre diffraction can be used to study aspects of polymer structure that can not be studied by x-ray methods - e.g. information on water or on the location of hydrogen atoms.

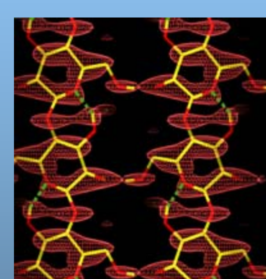
Biological polymers



Neutron fibre diffraction patterns recorded from DNA fibres hydrated with D2O (left) and with H2O (right). Intensity differences are observable throughout the entire diffraction range and can be used to locate structured water.

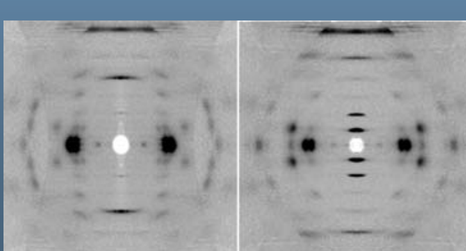


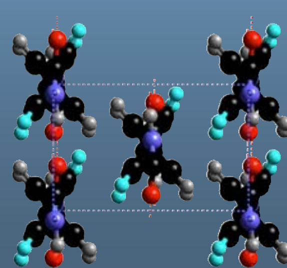
A-DNA hydration (Shotton *et al*, 1998)



Hydrogen bonding in cellulose (Nishyama *et al*, 1999; Langan *et al*, 1999)

Synthetic polymers





Revised structure for PPTA, based on neutron fibre diffraction analysis

Neutron fibre diffraction data recorded from selectively deuterated PPTA (known commercially as Kevlar) showing that the model structure, accepted from the 70's, is in need of modification (Gardner, Forsyth *et al*, in preparation)