



# Set-up and running a service

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# Why have a service?



- **For user:**
  - **Distance and cost**
  - **Small number of samples**
  - **No learning curve**
  - **Convenient**
  
- **For source**
  - **Good way of expanding user community**
  - **More efficient use of time**
  - **Well trained group**

# Types of service



- **Data collection.**
- **Data collection and processing.**
- **Data collection, processing and full structure refinement.**

# Services

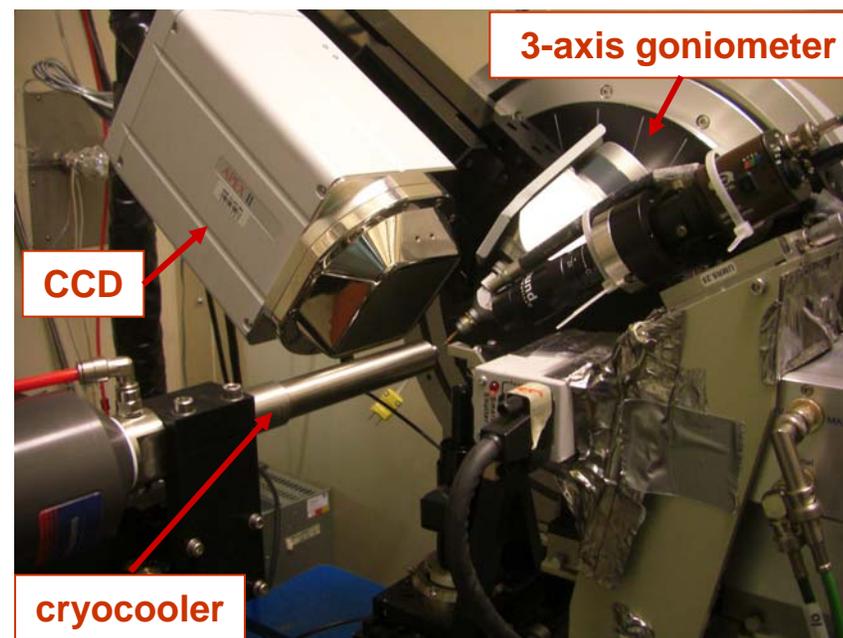


- **UK National Services (SRS and later Diamond)**
- **EU service (SRS)**
- **Industrial Service (DARTS)**
- **SCrALS (Service Crystallography at Advanced Light Source)**
- **SCrAPS (Service Crystallography at Advanced Photon Source)**

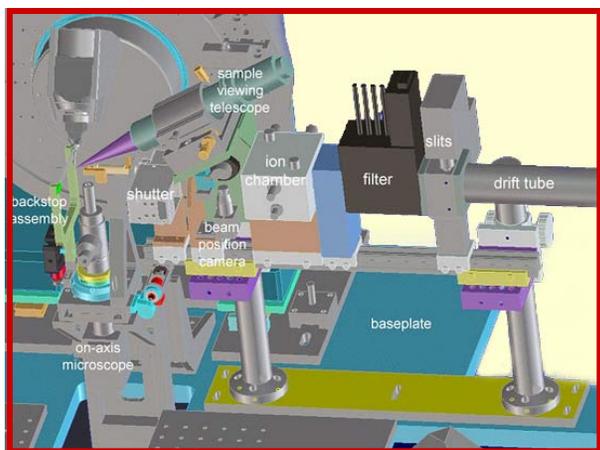
## 11.3.1 station



- Bruker AXS APEX II CCD detector (Fairchild), four-port readout.
- Equipped with a 3 circle, fixed-Chi ( $54.7^\circ$ ) Bruker goniometer.
- Typical exposure times:
  - for single crystal experiments: 0.5 to 5 s/frame.
  - for powder XRD: 120s/frame.

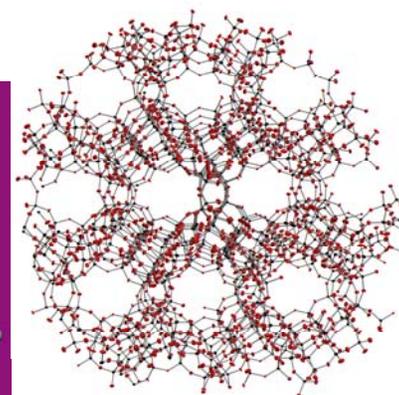
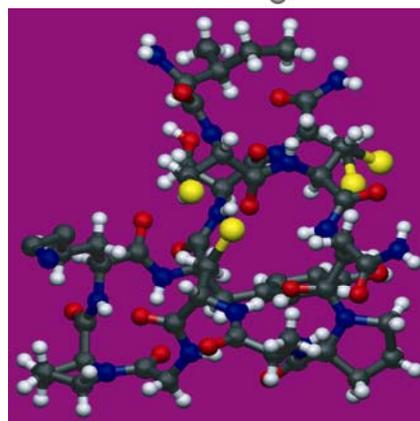
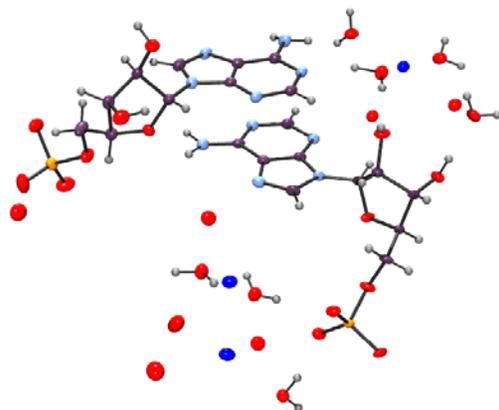
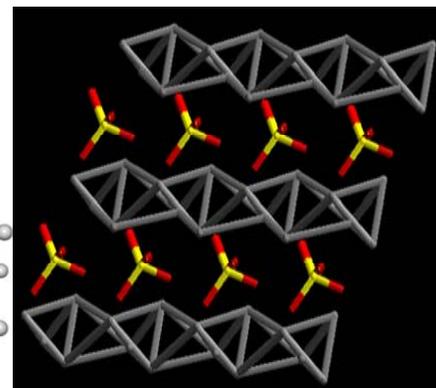
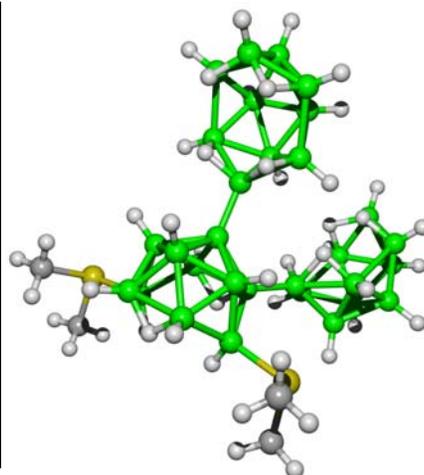
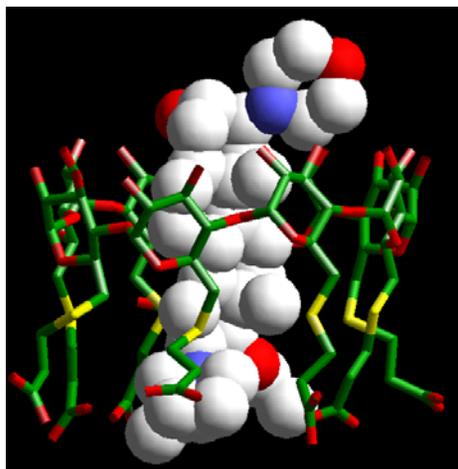


11.3.1 Endstation- Small Molecule Crystallography Set-up

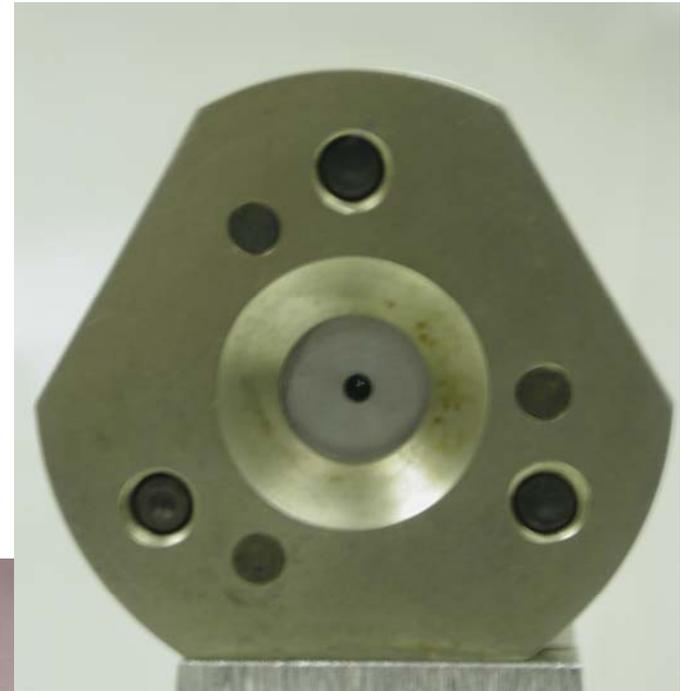
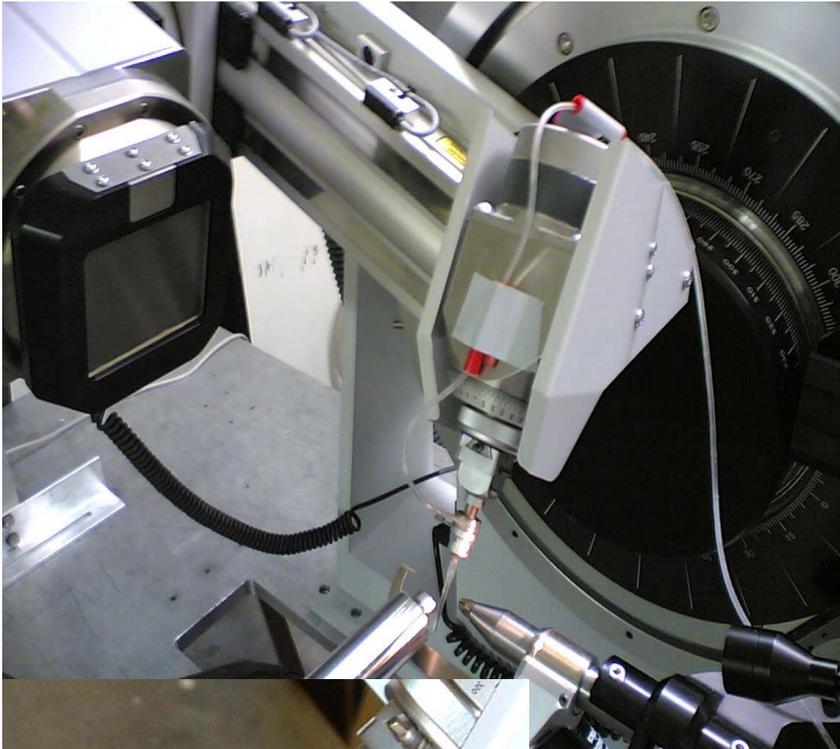


- The Bruker APEX2 software is used to resolve compound structures (Single crystal XRD).
- Smart or Fit 2D or Xmas are used to analyze the powder and high pressure XRD data.

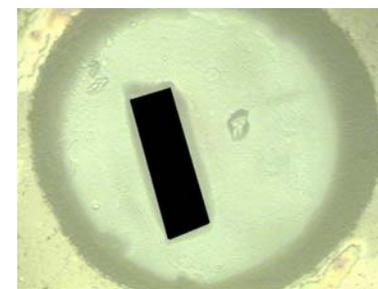
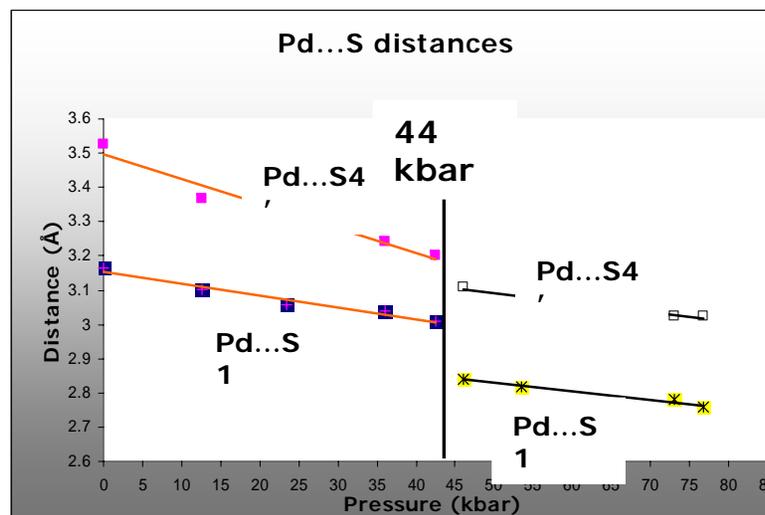
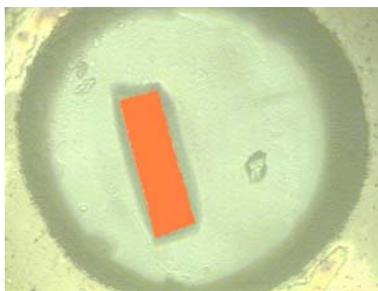
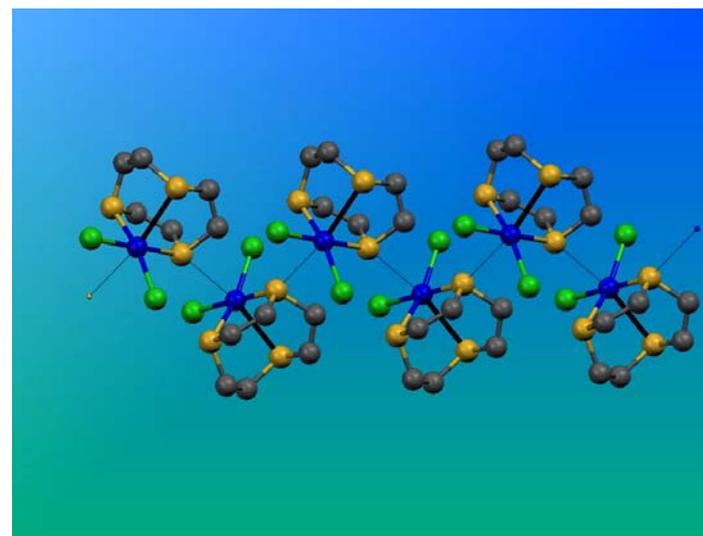
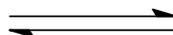
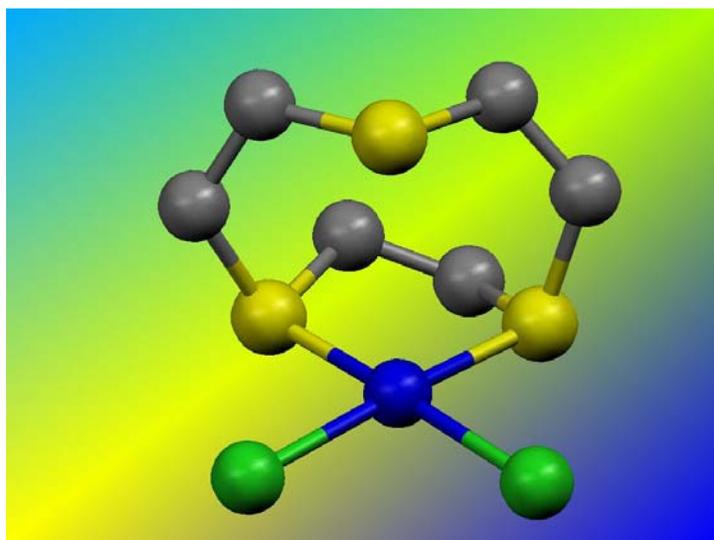
# Structures



# Environmental Cells



# High Pressure

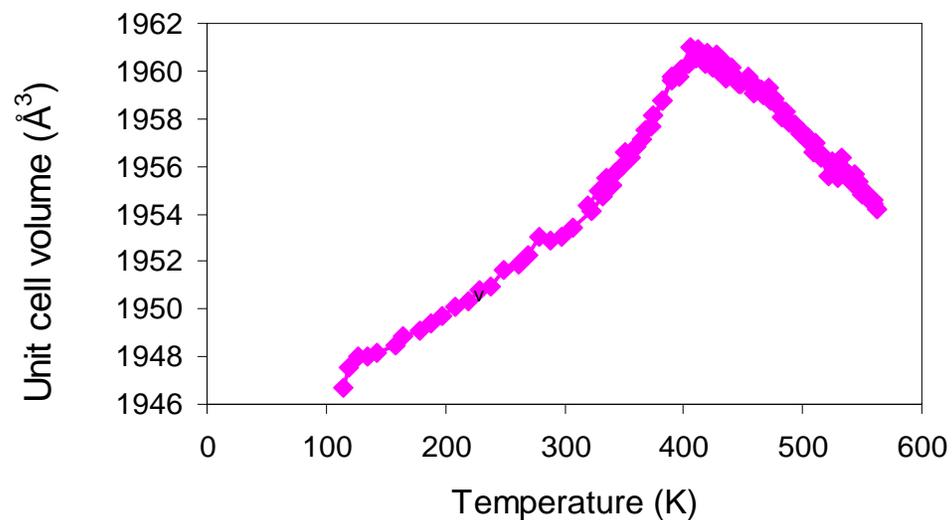
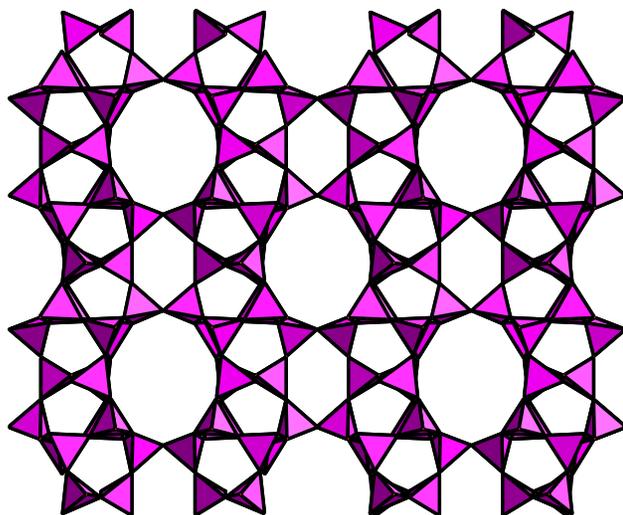


Allan et al *Chem. Comm* 4081- 4083, 2006

# Variable Temperature



- Thirteen data sets from 133 K to 513 K



Morris, *et. al.*, *J. Am. Chem. Soc.* 2001, **123**, 5453

Morris, *et. al.*, *J. Am. Chem. Soc.* 2003, **125**, 4342