Course structure - For convenience the work will be divided up into three parts and written up as three reports.

(i) Applications of the Cambridge crystallographic database (CCD) and associated software (Conquest, Vista, Mercury)

The TAs will guide the students on how to access the Cambridge Crystallographic Database using the laptops provided. A class exercise will then be carried out whereby each student is assigned a 1st row transition metal and asked to find out the typical geometries for the metal, including bond lengths when coordinated by a common atom e.g. oxygen as in EDTA complexes. Not quite as simple as it looks – oxidation state, tetrahedral, octahedral all influence the bond lengths. If things are going well, room for improvisation – choose another coordinating atom S, N …
Finish off by combining the bond lengths and angles from all the students to form a class dataset, so that comments can be made on any trend across the periodic table.

(ii) Crystallisation experiments

One of the most important steps in X-ray crystallography is growing a suitable crystal. The TA will guide small groups of students through the process of crystallisation by vapour diffusion and slow evaporation. To make the work more interesting metals and ligands will be mixed drop-wise to form complexes, which are then subjected to the vapour diffusion process. The students are expected to describe the products of their endeavours and assess the crystallisation methods.

(iii) Transforming a Crystallographic Information File (CIF) into an Acta Cryst. publication.

Each student will be given an unpublished Crystallographic Information File and will be expected to write a paper in the style of Acta Crystallographic C. This work will be carried out on the laptops provided and will build on the Cambridge Crystallographic Database skills developed in the 1st practical. The student will look for published crystal structures containing similar fragments to their CIF structure, which they can use to help write their own paper. The TA will assess the student's interpretation of their own crystal structure to ensure that the students are searching for the correct fragments. The TA will also provide guidance on the use of Mercury software to draw structures and PublCIF, which is used to convert the CIF data into a formatted publication. Guidance would also be needed to help the students understand non-bonded interactions such as hydrogen bonding and on how to illustrate these using Mercury.

It would be helpful if the TAs demonstrating on this course had some familiarity with using the data in CIFs to write reports or papers but not essential and tuition in the use of the above programs will be provided if required.

If a TA wanted to help with marking the reports, guidance would be given and remuneration provided at TA rates.