Oral presentation

We've seen it all: a service crystallographer's practical, creative advice to students of the art

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It is not practicable to write a meaningful "flow chart" for experimental crystallography. That is to say that each step on the way to determining a crystal structure, starting with crystal growth and ending with publication, has so many variables that any attempt to define a workflow chart would rapidly result in something with multiple overlapping options. It would be of no use at all. The (young?) trainee crystallographer generally learns by practice and repetition under the tutelage of an experienced mentor. Ideally this would be over a very broad range of chemistry so that as many problems as possible are encountered and handled as part of one's education.

However – and this is particularly true in chemical crystallography – students tend to focus on just their own experimental project work, leaving vast swathes of chemistry untouched. Some may get to their end of their studies without ever having handled an air- sensitive crystal or seen a twinned diffraction pattern. The really lucky ones might never have had to model disorder. Most will not have experienced the pleasure of identifying and mounting a really nice-looking crystal at 16:45 on a Friday only for the diffraction images to resemble a snowstorm, the nice-looking crystal now seemingly having been struck with a 100 Kelvin "sledgehammer" and the dawning realisation that the hoped-for 17:00 departure for the weekend is but a distant dream.

Service crystallographers, on the other hand, have generally seen it all. In a university setting we often work independently of research crystallography students, separate yet a fount of practical knowledge for all young crystallographers struggling with whichever problematic crystal happens to be mounted on the diffractometer. This talk will draw on almost 20 years of providing crystal structure analysis on a service basis to discuss a range of experimental crystallographic issues and offer some possible solutions so that the student crystallographer is better armed to tackle a bigger range of problems. How best to handle rapidly desolvating crystals… when they're an NMR tube (oh, and air-sensitive to boot)? What are the tell-tale signs of an unexpected phase transition, and what to do next? When the vial contains only one crystal, how do we get it out – and can we trust the results?