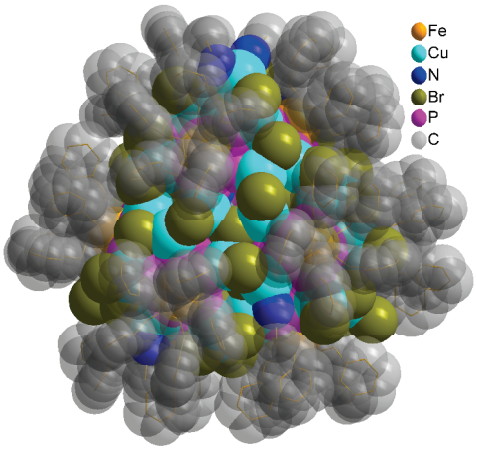

Figure 1. Supramolecule $[\{Cp^{Bn}Fe(\eta^5\text{-}P_5)\}_{12}\{CuBr\}_{51}\{MeCN\}_8]$ in 1, H atoms are omitted for clarity.

Keywords: X-ray single-crystal diffraction, data collection strategies, model refinement, disorder, unstable crystals

MS13-P5 Automated data analysis for X-ray diffraction experiments in chemical crystallography

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In chemical crystallography the routine use of fully automated data reduction (Winter & McAuley, 2011) is not as widespread as in the closely related field of macromolecular crystallography (MX). Data processing times are not crucial for data collection on laboratory sources and did not constitute the rate-limiting step for collections at the two dedicated small-molecule synchrotron beamlines worldwide. As data collection times decrease through advances in detector technology, processing times become more important.

Here we present the current progress in adapting and extending MX data analysis and reduction software to chemical crystallography applications, and implementing these in an automated data processing pipeline at the dedicated chemical crystallography beamline I19 at the Diamond Light Source (Nowell *et al.*, 2012). The beamline will, following an extensive hardware and software upgrade later this year, be equipped with a Pilatus 2M pixel-array detector. The concomitant reduction in data collection time and the expected increase in the volume of data collected necessitates a greater level of automation in terms of data processing and reduction. To achieve this goal MX software, such as GDA (General Data Acquisition framework; Gibbons *et al.*, 2011) used for data collection at DLS, the data reduction expert system xia2 (Winter, 2010) and the Diffraction Integration for Advanced Light Sources (DIALS) software suite, are modified and extended to accommodate chemical crystallography requirements.

In chemical crystallography data are commonly collected using spherical or hemispherical data collection strategies, which are comprised of multiple sweeps based on the rotation method. In the proposed setup the auto-indexing solutions are continually refined throughout data acquisition, and, based on the relevant current indexing solution and hitherto collected data, further data collection strategies are evaluated using DIALS, and subsequently proposed to the experimenter.

Diffraction data are processed in the background using xia2 and DIALS, which both run as modules in the Computational Crystallography Toolbox (cctbx; Grosse-Kunstleve *et al.*, 2002).

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Keywords: chemical crystallography, data reduction, automation