

Poster Presentation

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Effective data collection and refinement of pertubated structures

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Approaches to determining the influence of individual measurements on the precision of crystallographic least squares parameters have been known for a long while.[1] Situations in which the precision of a single parameter (or linear combination of parameters) is critical can include: determination of novel bond lengths; refinement of site occupancies in mixed metal or mixed oxidation state systems; determination of the fraction of excited state molecules in a time-resolved pump-probe experiment. Such calculations are easily applicable to point-detector instruments, where individual influential reflections could be remeasured one-by-one. However, on a modern area detector instrument many reflections are measured on one frame and therefore some consideration of the appropriate strategy of reciprocal space scans is permitted to allow a more efficient use of the instrument. The highly influential partial data collection is then feed into an appropriate refinement model. Occupancies in mixed-metal or mixed-oxidation state systems and fractions and positions of excited state molecules during a time-resolved pump-probe experiment can be determined using direct refinement of the perturbation of the structure from the ground state. Re-factoring to modern Fortran of the Crystals software is in progress to allow the implementation of new algorithms such as a difference refinement.[2] We present an analysis of diffractometer strategy selection to prioritize scans which give the best improvement in specific least-squares parameters and a novel algorithm for the refinement of the partial data using crystals.

[1] Rawlings J. O., Pantula S. G., Dickey D. A. (1998). *Applied Regression Analysis: A Research Tool*, 2nd ed. New York: Springer., [2] Vorontsov I., Pillet S., Kaminski R., et al. (2010). *J. Appl. Cryst.* 43, 1129-1130.

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