Poster Presentations

[MS31-P03] Alternative criteria for optimal data collection strategy

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Approaches to determining the influence of individual measurements on the precision ofcrystallographic least squares parameters have been known for a long while [1,2,3,4,5].Situations in which the precision of a single parameter (or linear combination ofparameters) is critical can include: determination of novel bond lengths; refinement ofsite occupancies in mixed metal or mixed oxidation state systems; determination of thefraction of excited state molecules in a time-resolved pump-probe experiment.Such calculations are easily applicable to point-detector instruments, where individualinfluential reflections could be remeasured one-by-one. However, on a modern areadetector instrument many reflections are measured on one frame and therefore someconsideration of the appropriate strategy of reciprocal space scans is permitted to allowa more efficient use of the instrument. We present an analysis of diffractometer strategy selection to prioritize scans whichgive the best improvement in specific least-squares parameters.

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