MS30 P01

Refinement of Crystal Structures with Pseudo-translational Symmetry Martin Lutz, Anthony L. Spek *Bijvoet Center for Biological Research, Crystal and Structural Chemistry, Utrecht University, The Netherlands.* E-mail: m.lutz@chem.uu.nl

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Due to the advances in X-ray diffractometers (area detectors) and the easy accessibility of low temperature units leading to solid-solid phase transitions, pseudotranslational symmetry is nowadays frequently observed in standard crystal structure determinations. The search algorithms in the SIR packages [1] and the ADDSYM routine of the program PLATON [2] are valuable tools to detect pseudotranslational symmetry. Simulated precession images as generated with the COLLECT suite [3] help to overcome indexing problems.
Much information about deviations from the average structure is contained in the weak reflections. Weighting schemes suggested by refinement programs, however, tend to down-weight weak reflections [4].
We will present a comparison of different refinement strategies and weighting schemes. Their influence on the stability of the least squares procedures and the results will be discussed with examples from small-molecule structures.

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MS30 P02

Fractal dimension as a tool for judging the quality of the residual density Kathrin Meindl, Julian Henn, *Institute of Inorganic Chemistry, University of Göttingen, Germany.*
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Keywords: fractal dimension, residual density analysis, box-counting algorithm

Residual density analysis is a very important criterion for the adequacy of the model and the quality of the fit in high resolution charge density refinement. Furthermore, being flat and featureless is a necessary condition for the residual density map [1]. Flatness can be evaluated by doing a peak search analysis of the map but featurelessness is so far only approved by visual inspection of individually selected planes containing the heaviest atoms. Thus, it would be desirable to have a continuous and bounded quantitative measure for featurelessness, which characterizes the whole unit cell.
We have developed a program to calculate the fractal dimension [2,3] of the residual density in the unit cell, which assigns a number between 0 and 3 to each residual density value depending on the frequency of its appearance. This was done by applying an advanced examination of the results received by a modified box-counting algorithm. The resulting residual density distribution reveals systematic limitations of the electron reconstruction process. Deviations from the ideal shape of the distribution hint towards shortcomings in data quality and modelling, e.g. disorder broadens the peak in the periphery. The fractal dimension is an appropriate tool for quantifying and analyzing the featurelessness of the residual density.

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