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Evaluating structures derived from X-ray powder diffraction data using entropy

D. Sisak Jung[1,2], L. McCusker[2], C. Baerlocher[2], C. Gilmore[3]

[1]DECTRIS Ltd, Baden, Switzerland, [2]ETH, Laboratory of Crystallography, Zurich, Switzerland, [3]University of Glasgow, School of Chemistry, Glasgow, UK

So far, in the field of X-ray powder diffraction, the maximum entropy method (MEM) has been used to (i) solve the phase problem, (ii) estimate the intensities of overlapping reflections, (iii) predict the intensities of missing reflections, and (iv) improve electron density maps generated during Rietveld refinement. We found a new application for MEM in a recent study, in which the powder charge flipping algorithm [1] in Superflip was applied to all-light-atom structures [2]. It proved to be difficult to identify the few fully interpretable maps within in the 200 generated in a typical Superflip job using the standard evaluation criteria. In 1992, Sato reported that entropy could be used as a solution evaluation criterion if the basis set is large, the phases are close to the correct ones, and the structure contains a small molecule [3]. Reasoning that these requirements would be fulfilled by the better Superflip solutions, all solutions were input to the MEM program MICE to calculate the corresponding ME maps and their entropies. Tests performed on several datasets showed no direct correlation between entropy and the solution quality. However, it was noted that a certain number of solutions show entropy values significantly lower than the others. This group usually contained one fully interpretable map. Refinement of the approach led to a relatively straightforward method for recognizing the better solutions. Furthermore, phase recycling based on this approach proved to be useful. As a result, guidelines for solving structures of different levels of complexity using the pCF algorithm could be devised.

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