

## **Walking the Tightrope of Complexity – Assessing Probability of Success of Structure Solution from Powder Diffraction Data**

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This presentation will attempt to outline some of the thought processes and logic that can contribute when answering the question ‘can you solve this?’ Answering this question with what can be a bare minimum of information (and sometimes none!) is always going to be difficult but a reasonable assessment of risk must nonetheless be made. Even where the complexity seems manageable there are always going to be occasions when a structure does something unexpected such as possessing a rare space-group or maybe the data exhibits a nasty microstructure. Some such problems can be identified and tackled given sufficient time but clients may not want to invest additional resources into something edging ever closer to a research project than a timely result.

The brute-force computational nature of real-space methods such as simulated annealing invite the use of code-breaking as an analogy. In code-breaking ‘cribs’ (or clues) are used to either point in the correct direction or exclude portions of search-space to reduce the computational requirements. Similarly in indexing and simulated annealing, key pieces of information such as absolute density, stereochemistry, water content, etc., can improve the chances of finding a solution in a reasonable amount of time given limited computing resources. Most researchers will have one or more apparently simple structures that should have solved readily but inexplicably refused to produce a satisfactory solution. However, a probabilistic approach is a good guide to assessing risk in a structure solution process. Good examples of this are the tables of space-group frequencies in the crystallographic literature produced via data mining from entries in the Cambridge Structure Database.

A real example will be used to demonstrate ways a problem can be assessed at different stages of the structure solution process, and how prior knowledge is leveraged to improve the probability of success within a manageable timescale.