# Improved crystal structure solution from powder diffraction data by the use of conformational information

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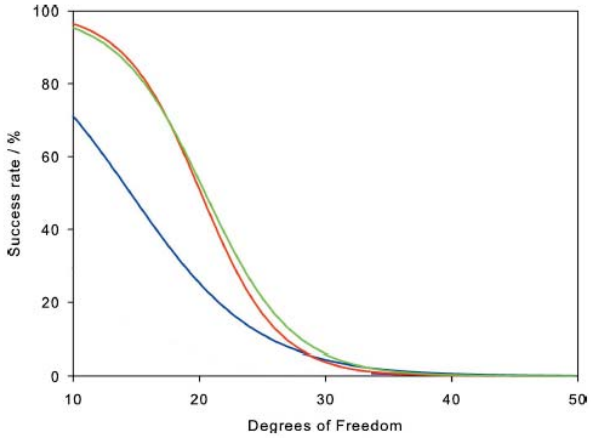
Crystal structure determination from powder diffraction data has benefitted tremendously from the use of global optimization methods. Many computer programs (including, but not limited to, *DASH*, *EXPO*, *PSSP*, *TOPAS* and *FOX*) implement global optimization in the form of simulated annealing and have been used to solve many complex crystal structures from powder data alone [1]. Key to the success of this type of approach to structure determination is the inclusion of significant amounts of prior chemical knowledge in the form of the known molecular connectivity of the structure under study. Any torsion angles around which atoms are free to rotate are generally treated as variables to be determined by the optimisation procedure and are allowed to vary freely in the range of 0–360°. Here we report on the improved performance of global optimization in the *DASH* computer program *via* the implementation of conformational restraints, or conformational bias, derived from crystal structures stored in the Cambridge Structural Database (CSD) [3] to these freely varying torsion angles.

Fifty-one PXRD datasets, collected from organic molecules spanning a large degrees-of-freedom range were assembled. Fifty DASH runs, using optimized parameter settings [4] were performed on each dataset. These runs were then repeated, but with the application of either (a) a modal constraint derived from the *Mogul* library of the CSD or (b) a distribution bias derived from *Mogul*, to any freely varying torsion angle in a structure. An empirical log-of-the-odds (ELO) analysis was performed in order to evaluate any increase in the success rate of solving a crystal structure as a result of introducing conformational information via *Mogul*.

The figure to the right shows the significant improvement obtained using either Mogul (red middle line) or Mogul distribution bias (green upper line) compared to default *DASH* success rates in solving crystal structures (blue lower line). Improvements are evident over the entire range of degrees-of-freedom present in the PXRD datasets. This enhancement allows problems of greater molecular complexity to be tackled as a result. Whilst the *Mogul* constraint and distribution bias approaches yield similar benefits, the fully automated distribution bias approach is particularly attractive.




It is likely that other global-optimization-based approaches to SDPD can benefit from this type of prior information, and the tools provided in the CSD are extremely valuable in this regard.

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**Keywords: simulated annealing, molecular structures, conformational bias**