K5 **Statistical Methods in Protein Crystallography**. Randy J. Read, Airlie J. McCoy and Laurent C. Storoni, *Department of Haematology, University of Cambridge, Cambridge Institute for Medical Research, Wellcome Trust/MRC Building, Cambridge CB2 2XY U.K.*
E-mail: rjr27@cam.ac.uk

Keywords: Maximum likelihood; Experimental phasing; Molecular replacement

Most algorithms for macromolecular crystallography have been based traditionally on either least-squares optimisation or analysis of the Patterson function. In recent years, great progress has been made by reformulating these algorithms in terms of the principle of maximum likelihood. The basic idea behind likelihood is fairly simple: the quality of a model is judged by the probability that model assigns to the set of observations that was measured. If the errors in predicting the observations from the model are Gaussian and arise only from measurement error, likelihood is equivalent to least-squares. Many probability distributions relevant to crystallography are indeed Gaussian, but they describe the relationships among phased structure factors. Elimination of the unknown phase changes the form of the distribution so that it is necessary to apply a proper maximum likelihood treatment, instead of simply using least squares. Some likelihood-based methods are very slow, but reasonable approximations can be computed quickly. Interestingly, some of these approximations turn out to bear a close relationship to Patterson-based methods.

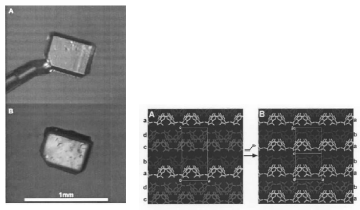
Likelihood has now been applied to a number of areas in protein crystallography: the estimation of model phase probabilities and computation of map coefficients in the program *SIGMAA*; the refinement of atomic models in *CNS*, *Refmac* and Buster/TNT; experimental phasing in *Sharp*; molecular replacement in Beast. We have been developing a new program for likelihood-based phasing in macromolecular crystallography. Our program, *Phaser*, implements new methods for solving structures by molecular replacement, and new methods for experimental phasing are under active development.

In my talk, I will describe the current capabilities of *Phaser*: anisotropic normalisation, likelihood-based fast rotation and translation functions, MIR phasing and SAD phasing, and I will show how some difficult structures can now be solved easily. I will discuss some of our future plans to increase the sophistication of *Phaser,* particularly in accounting for correlations in sources of error and in combining the information from molecular replacement and experimental phasing.

K6 **Self-Reassembly in the Organic Solid State.** Jerry L. Atwood[a], Leonard J. Barbour[b] and Ágoston Jerga[c], *University of Missouri-Columbia[a,c], USA and University of Stellenbosch, South Africa[b]. E-mail: atwoodj@missouri.edu*

Keywords: Self-assembly; Porosity; Phase Transformation

More than 800 papers have been published on p-tert-butylcalix[4]arene. However, we have recently discovered that this well-known macrocycle undergoes single-crystal-to-single-crystal phase transitions upon guest uptake and release. The calixarene does not possess pores or channels in the solid state. However, despite a lack of porosity of the material, guest transport through the solid occurs readily until a thermodynamically stable structure is achieved. In order to actively facilitate this dynamic process, the host molecules undergo significant positional and/or orientational rearrangement. This transformation of the host lattice is triggered by weak van der Waals interaction between the molecular components. In order for the material to maintain its macroscopic integrity, extensive cooperativity must exist between molecules throughout the crystal, such that rearrangement can occur in a well-orchestrated fashion. Implications of this discovery for gas separation and gas storage will be discussed.



[1] Atwood, Barbour, Jerga and Schottel, (2002) *Science*, **298**,1000.