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A Recent Advance in the Direct Methods of Phase Determination. Hongliang Xu, Charles M. Weeks, Herbert A. Hauptman, David A. Langs, Hauptman-Woodward Medical Research Inst. & Dept. of Structural Biology, SUNY at Buffalo, 73 High St., Buffalo, NY 14203.

The phase problem of X-ray/neutron crystallography may be formulated as a problem in constrained global minimization. A new type of minimal function, based on the statistical distribution of structure invariant values, serves as the foundation of an optimization procedure called statistical *Shake-and-Bake*.

Favorable application of this procedure to phase determination depends on the choice of the statistical interval. The effects of interval variation have been studied for the structure of cyclosporin (neutron) and 19 selenium-atom substructures (X-ray), and the results have shown overall improvement in success rate relative to traditional *Shake-and-Bake*. Statistical *Shake-and-Bake* is being incorporated as the default optimization procedure in newly distributed versions of the *SnB* and *BnP* computer programs.

This research was supported by NIH grants EB002057 and GM072023.