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Novel Statistical Approach to the Phase Problem. Hongliang Xu, Herbert A. Hauptman, Hauptman-Woodward Medical Research Inst. & Dept. of Structural Biology, SUNY, Buffalo, NY.

The phase problem of X-ray crystallography may be formulated as a problem in constrained global minimization. The minimal function and its minimal principle employed in the traditional *Shake-and-Bake* algorithm rely on the probabilistic estimates of the cosines of the structure invariants. A novel statistical approach to the phase problem, which utilizes statistical properties of the structure invariants, has been recently proposed. The statistical minimal function and its minimal principle are formulated, and the corresponding statistical *Shake-and-Bake* algorithm and its associated statistical parameter-shift procedure are proposed and tested.

The test results, based on 20 selenium-atom substructures spanning different sizes, resolutions and space groups, show that the statistical approach to the phase problem is a simple, reliable, less computationally intensive and more efficient procedure for phase determination in X-ray crystallography. The Statistical *Shake-and Bake* method has been incorporated into the latest versions of computer programs *SnB* and *BnP*.

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