Structure Determination from a Quantum Mechanical Formulation in Momentum Space

Kostas Bethanis[a], Athanassios Hountas[a], Pavlos Tzamalis[a], Georges Tsoucaris[b], [a]*Department of Sciences, Agricultural University of Athens, Greece.* [b]*Laboratoire de recherche des Musées de France, Paris, France.* E-mail: kbeth@aua.gr

The proposed method aims at the crystal structure determination by using the theoretical background of quantum mechanics. This is achieved through the quantum mechanical formulation in momentum space by means of the Fourier Transform (FT) of the usual Schrödinger equation in direct space. The key step is the identification of the FT of the potential function V(r) with the expression $E(H)/H^2$ where E(H) is the normalized structure factor. An algorithm has been developed for practical implementation of this new method for direct phasing of x-ray data [1]. In this algorithm a new criterion, based on the crystallographic symmetry, has been introduced. The idea consists of testing the phase calculation, extension and refinement, by deliberately sacrificing the space group symmetry information and using its gradual re-appearance as a criterion of correctness [2].

New theoretical developments relevant to the convergence of this algorithm in different cases have been formulated. An upgraded algorithm for macromolecules has also been developed and tested in phase extension and refinement with promising results.

[1] Bethanis K., Tzamalis P., Hountas A., Tsoucaris G., *Acta Cryst.*, 2002, **A58**, 265-269. [2] Tzamalis P., Bethanis K., Hountas A., Tsoucaris G., *Acta Cryst.*, 2003, **A59**, 28-33.

Keywords: algorithm, phase problem, quantum mechanics