s8b.m2.p1 **Direct structure solution by a pair-functional method with self-consistent fields.** A.D. McLachlan, *MRC Laboratory of Molecular Biology, Hills Road, Cambridge, CB2 2QH, England.* e-mail: *admcl@mrc-lmb.cam.ac.uk*
Keywords: pair-functional, self-consistent field, direct method.

The Pair-Functional method[1] for solving molecular structures starts from a many-body statistical ensemble in the unit cell in which there is a eriodic pairwise additive effective potential energy between every pair of atoms. This Pairing Potential is a long-range energy function that depends on the relative distance and direction of any two coupled atoms. Its form is eternined uniquely by the X-ray intensities of the crystals, and is well approximated by the Ornstein-Zernicke direct correlation function of the corresponding ensemble.

Given the pairing potential, the method tries to solve the structure by a search for trial atomic arrangements that have the highest total pairing potential, and match the observed X-ray intensities.

The most promising search procedure tested so far is a temperature-dependent self-consistent field refinement. The ideal model system is an adjustable set of localised non-overlapping spherical cavities, cattered through the cell. Each cavity is able to contain no more than one atom, fixed at its centre. The pairing potentials act between centres and the occupancy of each cavity obeys Fermi-Dirac statistics. We seek thermal equilibrium at each centre subject to the mean long-range pairing field generated locally by all the other atoms. The model is solved by maximising an effective free energy function, under a carefully regulated regime of temperature control, while he cavities are also allowed to move. As the temperature falls the atom distribution condenses into a definite trial structure which improves progressively.

A simplified form of the model, which is easier to solve, but less accurate, represents the atoms as point-objects with variable occupancies, laid out on the vertices of a fine grid. Examples of small molecule and peptide structure solutions with 100-200 atoms will be shown.

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s8b.m2.p2 **Diffraction Image Simulations of Single TBSV Particles.** A. Zuev[*], P. Daniels[*], J. Hajdu[**], R. Neutze[**], D. van der Spoel[**], E. Weckert[*], R. Wouts[**]. [*]*Inst. für Kristallographie, Universität Karlsruhe (TH), Kaiserstr. 12, D-76128 Karlsruhe, Germany.* [**]*Department of Biochemistry, Uppsala University, Box 576, S-75123 Uppsala, Sweden.*
Keywords: methods crystallography, phasing, structure solution.

In previous studies elastic scattering of intense X-ray pulses from a single TBSV particle was investigated[1].

The main aim of the present studies was additional investigations taking into account also the second component contributing to a diffraction image of the viruses namely RNA which is confined to radii between 80 Å and 110 Å[2,3].

The molecular weight of RNA is known to be $1.5 \cdot 10^6$ that corresponds to approximately 4800 bases[2]. Little information exists on the three-dimensional structure of the RNA.

The following model was used for the calculations. The RNA was constructed from 215 molecules of RNA using PDB-entry 435D[4] distributed in a layer with middle radii (i) 90 and (ii) 80 Å with random orientations; this gives the corresponding molecular weight and number of bases. A comparison of the diffraction images with and without RNA was carried out. The calculations were made for low (20 Å) and high (2 Å) resolution. It was shown[1] that the number of scattered photons at high resolution is too little to give a significant diffraction pattern and it is necessary to average numerous scattering images from reproducible samples.

The possibility of using low resolution-diffraction image information where sufficient scattered photons are available for the numerical analysis of the orientation is discussed. To decide whether the image patterns contain sufficient information to numerically orientate the molecules the correlation function between patterns with different orientations will be discussed taking into account the expected diffraction signal.

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