s8b.m1.p8.la **A novel free-mounting system for protein crystals: transformation and improvement of diffraction power by accurately controlled humidity changes.** R. Kiefersauer[1], H. Dobbek[1], S. Grazulis[1], M. Than[1] and R. Huber[1]. *[1]Max-Planck-Institut für Biochemie, am Klopferspitz 18a, D-82152 Martinsried.*
Keywords: cryocrystallography, crystal improvement, capillary-free mounting.

The large size and the irregular shape of the protein molecules mean that protein crystals are characterized by very slight lattice forces. They have high solvent content in the region of 30 to 70% or even as much as 90%. Consequently, protein crystals are often unstable, poorly ordered and restricted to characteristic crystal sizes between some μm to 1 mm. One effort revealing suitable crystals is to exchange the crystal solution via diffusion.

A novel device for capillary-free mounting of protein crystals is described. A controlled stream of air allows an accurate adjustment of the humidity at the crystal. The crystal is held on the tip of a micropipette. With a video system (CCD-camera), the two-dimensional shadow projections of crystals are recorded for optical analysis. Instead of the micropipette, a standard loop can also be used.

Experiments and results for different crystal systems demonstrate the application of this method, also in combination with shock-freezing, to improve crystal order. Working with oxygen-free gases offers the possibility of crystal measurements under anaerobic conditions. Furthermore, the controlled application of arbitrary volatile substances with the gas stream is practicable. The control of the environment of the protein crystal in combination with accurate optical and X-ray measurements on the crystal system offers enormous possibilities for fine-tuned crystal engineering.

s8b.m3.p4.la **Spherically averaged phased translation function and its applications to search of molecules and fragments in the macromolecular electron density maps.** A. Vagin1 and M. Isupov2, *1Department of Chemistry, University of York, Heslington, York YO1 5DD, UK; alexei@ysbl.york.ac.uk, 2School of Chemistry, University of Exeter, Stocker Road, Exeter, EX4 4QD, UK.*
Keywords: methods crystallography, refinement, modelling.

In some cases it is difficult to solve an X-ray structure by molecular replacement even when structure for some homologous molecule is known. If prior phase information either from SIR/MAD or from prepositioned partial structure is known then it could be used in the six dimensional search programs like ESSENS[1], FFFEAR[2] to find the remaining part of the molecule or its fragment.

We suggest a new approach which divides six dimensional search with phases into three steps. First spherically averaged translation function is used to locate position of the molecule or its fragment. It compares locally spherically averaged experimental electron density with that calculated from the model and tabulates highest scoring positions. Then for each such position local phased rotation function is used to find the orientation of the molecule. Third step is the phased translation function for found orientation which checks and refines the found position.

This method has been implemented in the program MOLREP[3]. The technique has been successfully applied to locate molecules and α-helices in several test cases.

This technique could also be used to superimpose distantly related molecules. It uses FFT on all stages which means that it is fast and the time required is comparable to conventional molecular replacement searches. The program MOLREP is available free from A. Vagin, anonymous ftp account: ftp.ysbl.york.ac.uk or from CCP4. Details of the algorithm and examples of its application to real structures will be presented.

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