12.1–4 RESULTS OF CRYSTALLOGRAPHIC STUDIES OF THE 3-FE FERREDOXIN (FDII) OF Desulfovibrio gigas.

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Ferredoxin from D. gigas has been isolated in several aggregated states, two of which have been extensively studied at pH 7.6. FdI is a trimer of the protein unit (M_r=6400) with 4Fe-4S centers and redox potential of -455mV. FdII is a tetramer with 3Fe-4S centers of potential -130mV. FdI serves in electron transport in the phosphoroclastic reaction whereas FdII mediates electron transport between cytochrome C3 and sulfite reductase. It is now known that interconversion between 3Fe and 4Fe centers can occur in several Fe-S proteins.

It has been possible to crystallize the more stable FdII at pH 5.0 and 23°C. The space group is C2 with cell parameters: a=40.8Å, b=45.0Å, c=26.5Å, β=104.6°. The best crystals grow at 23°C rather than 0°C; no measures were taken to assure anaerobic conditions. The ratio of cell volume to monomer weight is 1.84, suggesting that the molecule can be no larger than a dimer (with 2-fold symmetry) but is more likely the monomer unit.

Reflection intensities comprising both Friedel pairs have been collected to 2.5Å. The Patterson map using 1214 anomalous differences gives clearly defined peaks which can be fit by a 3 iron cluster. Preliminary refinement against the 270 largest Bijvoet differences gives interatomic distances ranging from 3 to 4Å.

Progress in determining the structure of this iron-sulfur protein will be presented.

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12.1–5 ON THE USE OF A GUINIER FILM SCANNER SYSTEM.

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Experience with a microcomputer controlled Guinier film scanner system will be discussed. A single-beam microdensitometer using as measuring unit an IR emitting diode (λ=940 nm), a collimator and photodiode has been used for analytical and structural studies during the last three years. In order to avoid stray light, lens aberrations and focusing problems optical components such as lenses, prisms or mirrors are avoided (Johansson, K-E., Palm, T. and Werner, P.-E., J. Phys. E: Sci. Instrum., 13 (1980) 1289).

A modular computer program structure makes it possible for the operator to control all steps in the data evaluation. It is concluded that "black-box" evaluation of photographs may be used for analytical search-match studies, but can not be recommended for the low angle lines in indexing work. Transmitted light beam intensity is more sensitive than optical density data for investigation of weak diffraction lines. The human eye, however, is still the most sensitive instrument for pattern recognition. An essential part of the evaluation system is therefore a plot program, to aid visual inspection of the photograph. The most accurate positions of very weak lines can be determined by the internal standard technique using the plot program. Usually $\Delta(2\theta)$ is less than 0.01°. As the zero point error is included in this figure, the efficiency of the trial-and-error indexing program, TREOR (Werner, P.-E.) is high.

Although it is possible to find extreme high symmetry, test samples where a very small step-scan width may improve the accuracy, it is concluded that a collimator opening less than 0.04 mm is too small for ordinary practical problems.

A correction procedure for the non-linear relation between exposure and optical density makes it possible to use one single photograph for analytical and structural work.

The conclusion will be illustrated with data from structure determinations of for example Mg_2NiH_x ($0 \leq x \leq 4$), $Cs_2V_4O_{11}$ and unstable compounds such as $Na_2S \cdot 2H_2O$.

12.1–6 AN INTERACTIVE MICRO-COMPUTER PROGRAM FOR EVALUATION OF X-RAY POWDER FILM DATA

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A Line-Scanner (Johansson,K.E. et al., J.Phys.E: Sci.Instrum. 13 (1980),1289), has been used for measuring the optical transmission of Guinier X-ray powder diffraction films. Data are recorded in steps of 0.04 mm (0.0115° in θ) and fed to a microcomputer with graphics (240x240 addressable pixels).

Transmission data are converted to intensity values, and the intensity profile is displayed on the screen, permitting fast and detailed visual analysis of the recording. Peak positions and background settings are provided by automatic routines, but the operator can manually apply additional corrections of the background setting, remove spurious peaks, define peak widths etc. Integrated intensities and Bragg angles are finally calculated (use of internal calibrant can be included).

The results, together with the complete intensity profile data, are stored on floppy disk files. Facilities for further data analysis using standard crystallographic programs are provided by connection of the microcomputer to a larger host computer.