01.1-02 CRYSTALLOGRAPHIC STUDY ON STAPHYLOCOCCAL EXFOLIATIVE TOXIN. By C.S. Yoo, D.S.C. Yang, B.C. Wang and M. Sax. Biocrystallographic Laboratory, VA Medical Center, Pittsburgh, PA 15240 and the Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260, A. Johnson and L. Spero, Pathology Division, U.S. Army Medical Research Institute of Infectious Diseases, Frederick, Md 21701.

Exfoliative toxin, a protein with M.W. of 26,000 is known as an etiological agent for the Staphylococcal Scalded Skin Syndrome. Exfoliative toxin was first crystallized in space group $P2_1$ (Form 1) (Yoo et.al. J. Mol. Biol. (1978)124. PP. 421.) and later in $B2_1$ (Form 2). It was found that Form 1 can be transformed into Form 2 by altering solvent conditions. An interesting aspect of Form 1 is that it can be regarded as pseudo $B2_1$. The two molecules in the asymmetric unit of Form 1 are separated by a translation of 0.4 and 0.5 unit cell lengths along the x and z directions respectively. This information is obtained from the studies of a native Patterson map and an analysis of the intensity distribution. An isomorphous heavy atom derivative containing K_2PtCl_4 has been prepared. The usefulness of this derivative is being evaluated presently.

01.1-03 EXTRACTION OF DIFFRACTED X-RAY INTEGRATED INTENSITIES FROM WEAK PROTEIN DATA SETS. By J. Sygusch, Dept. of Biochemistry, Faculté de Médecine, Université de Sherbrooke, Sherbrooke, P.Q. Canada, J1H 5N4.

If the diffracted beam profile is analyzed in terms of a series expansion of generalized Hermitian polynomials the integrated intensity can be represented as the normalizing coefficient of this expansion. If the diffracted beam shape is independent of intensity, then by determining the shape function from a sufficient number of strong intensity profiles, the determined shape profile can then be used to analyze the weak intensity profiles. Errors due to intermittent noise during the profile measurement especially of weak data are considerably reduced. If analysis of the integrated intensity is carried out in terms of $|F|$ instead of $|F|^2$ the problem of handling negative integrated intensities such as in electron density calculations are resolved. The expression for the variance of $|F|$ is finite even for zero integrated intensity.

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01.1-04 MACROMOLECULAR CRYSTALLOGRAPHY WITH AN AREA DETECTOR USING CONVENTIONAL AND SYNCHROTRON RADIATION SOURCES. R. Kahn, R. Fourme and R. Bosshard, Laboratoire de Physicochimie Structurale, Université Paris Val de Marne, 94010 Créteil and LURE, CNRS - Université Paris Sud, 91405 Orsay - France.

An electronic diffractometer based on a spherical drift proportional chamber (Kahn et al, Nucl. Inst. and Meth. (1980), 172, 337-344) has been achieved and a software package for on-line collection of diffraction data from macromolecular crystals has been implemented and tested. The main characteristics of the detector are : simultaneous, parallax free, collection of data to a resolution of 1.95 Å at a typical wavelength of 1.40 Å, maximum count rate 3.7×10^5 cps, number of picture elements 10^5, quantum detective efficiency 0.6 at 1.4 Å. The detector is coupled to a modified rotation camera. The whole set-up is controlled by a minicomputer interfaced to a CAMAC-based data-acquisition system.

Reflection intensities are extracted from a sequence of electronic pictures. These pictures are optionally stills as in the method developed by Xuong et al. (Acta Cryst., 1978, A34, 289-296) or rotation pictures over small, contiguous, angular intervals. The second method is preferred for operation with the highly collimated synchrotron radiation source. The incident beam is monitored ; measurements are accordingly rescaled. Typical R_{sym}-values on intensities of symmetry related reflections obtained with a sealed X-ray tube and test crystals of beryllium acetate and gramicidin-A are ~ 5 %.

The diffractometer is currently being installed on the synchrotron radiation beam port D15 at LURE-DCI together with a tunable channel-cut monochromator. We aim at deriving phase information from anomalous scattering measurements at several wavelengths.

01.1-05 A METHOD FOR FAST AND ACCURATE COLLECTION OF X-RAY DATA FROM MACROMOLECULES. By B.O. Söderberg, Department of Chemistry and Molecular Biology, Swedish University of Agricultural Sciences, S-750 07 Uppsala, Sweden.

A method for fast and accurate collection of X-ray data from macromolecules using a 4-circle diffractometer is described. The method is intended to minimize the errors introduced in the integrated intensity when using the abbreviated ω-scan technique on a diffractometer not being optimized for that type of scan. The following two observations are utilized: 1) the width at half peak height of a reflexion is dependent on the χ and ϕ setting of the diffractometer; 2) the background is dependent on 2θ, χ and ϕ.

In accordance with these findings, the reciprocal space is divided into boxes of 2θ, χ and ϕ, and within each box the background and the width at half peak height are regarded as constants. Data are collected in a two pass procedure. In the first pass a few reflexions in each $2\theta,\chi,\phi$-box are measured. The background and the ratio between integrated intensity and peak height are stored. This ratio is closely related to the width at half-peak height.

In the second pass only the peak height is measured, and the net integrated intensity is calculated using the mean values of background and ratio stored in the appropriate box. This procedure drastically reduces the data collection time without appreciable loss of accuracy.