18.1-3 A FLEXIBLE PROCEDURE FOR THE ELIMINATION OF MANUAL RE-INPUT OF CRYSTAL STRUCTURE DATA. By K. Osaki, Nampei-dai 5-9-6, Takatsuki, Osaka 569, Japan, T. Taga, Faculty of Pharmaceutical Sciences, Kyoto University, Sakyo, Kyoto 606, Japan, and N. Yasuoka, Himeji Institute of Technology, Shosha, Himeji, Hyogo 671-22, Japan.

The usual procedure of publishing crystal structure results is to print the numerical data on paper, which are then re-input into the computer at data centers. This procedure involves manual input at two stages, which is a possible source of error and is undesirable also from the point of input cost.
A flexible procedure has been devised which helps authors to produce a computer-readable data set in standardized format. Its central part is a FORTRAN program to be run within the main-frame computer used for the structure analysis, which extracts prescribed data automatically and writes a file in standardized format (SCFS-87). Only the subroutine for extracting data must be modified so as to conform with the local program system. The output file, after manual editing if desired, may be copied onto any form of computer-readable medium, including 9-track standard magnetic tape. The problem of standardization of the record on 5-inch floppy disks was overcome in our case by use of the format defined by MS-DOS.

18.1-4 NRCVAX AN INTERACTIVE CRYSTAL STRUCTURE SYSTEM By E.J.Gabe, Y.Le Page, P.S.White and F.L.Lee, Chemistry Division, National Research Council of Canada, Ottawa, Canada K1A 0R9 and Chemistry Department, University of New Brunswick, Fredericton, N.B., Canada E3B 6E2.

The NRCVAX program system (Gabe E.J., Le Page Y. and Lee F.L., Crystallographic Computing 3, p. 167, 1985) is an integrated set of routines for the interactive solution, refinement and presentation of crystal structures from diffraction data. It has been expanded and made more consistent and easy to use. Terminal interaction is through many menus and a free-format input routine, which filters the incoming character strings to limit typing errors. New facilities include bestplane Fourier routines, a distance - angle routine which produces tabular output in a form suitable for publication and the routine MISSYM (Le Page Y. Abstract V6, ACA Meeting, June 1986) to detect missing symmetry in sets of atomic coordinates. There is a new routine to allow reflection data from non-standard sources to be put into the system easily. The structure solution routine SOLVER, which is loosely based on an early version of MULTAN, has been expanded and speeded up and MULTAN80 is also incorporated. A rigid-body least-squares refinement routine is being written. Graphics facilities have been greatly expanded and are now driven by an internal plotting routine. Contour plotting is included in all Fourier routines and the well-known graphics routines, PLUTO and ORTEP, are both available in interactive form. This allows easy generation and manipulation of mono- and stereo-plots. A great deal of effort has been expended to make NRCVAX F77 compatible and less VAX specific. The system is now running on SUN workstations and WICAT minicomputers. It should be adaptable to any 32-bit system, using virtual memory and ASCII and work has started on a PC version. The system can be very easily installed on a VAX and is available at no charge.

18.2-1 EXTENSION OF THE XTAL SYSTEM OF CRYSTALLOGRAPHIC SOFTWARE FOR PROTEIN CRYSTALLOGRAPHIC APPLICATIONS, Keith D. Watenpaugh*, Debra R. Holland*, and James M. Stewart†, *Physical and Analytical Chemistry, The Upjohn Company, Kalamaoo, MI and †Department of Chemistry, University of Maryland, College Park, MD, USA

The XTAL[1] system is a collection of programs designed to perform calculations necessary for the solution, refinement and analysis of crystal structures by diffraction techniques. The system is programmed in a Fortran77-like preprocessor, RATMAC, which transforms the code into local Fortran for maximum portability. The routines are invoked using a free-format control line interface which supplies the appropriate calling mnemonics and parameters to define the desired calculations. Crystal data is stored in a binary data file (BDF) which serves as a repository for all data pertaining to a given crystal structure analysis. The efficient and flexible structure of the BDF mechanism allows for dynamic modification of its logical records by any of the system routines. An additional collection of crystallographic routines for protein crystallography has evolved as an extension of the original XTAL system and is based on the same design philosophy and interface technique.

Among those routines included in "PROXTAL" for data reduction are: PROFIT, which fits diffractometer step data and background[2]; ABSCAL, which calculates and applies corrections for crystal deterioration and empirical absorption; and CRITIQ, which analyses the data for possible errors. Routines for using heavy atom isomorphous data include: FINDKB, which scales derivative data to native taking advantage of anomalous scattering[3]; BFOURR, which calculates various coefficients for the Fourier and other routines; and MIR, which calculates phases by either a modified Blow-Crick or a Sygusch-Bricogne procedure[4]. MAKBRK and PROATM provide interface with the FRODO system and the Brookhaven Protein Data. PRECED and CEDAR do crystallographic refinement combined with energy minimization and dynamics[5] and a generalized version of the B.C.Wang phasing routines is being converted[6]. Other programs are being considered for inclusion.

All programs are extensively documented both inside the code and in the manuals, allowing for further development by the user community rather than maintaining a static system.

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