intensities. For the estimation of the e.s.d.'s of the intensities, the spread of symmetry-equivalent data about a mean value may be used (recommendation 3 of the report); this spread will change in the course of the refinement, and the corresponding e.s.d.'s may have to be adjusted. In addition, derivatives of transmission factors with respect to crystal form parameters must be periodically updated. Thus, data-processing and refinement programs will be executed in turn. For the programming already accomplished see E. Blanc, H. D. Flack and D. Schwarzenbach (this conference).

MS-02.01.04 TRENDS IN PROTEIN CRYSTALLOGRAPHIC COMPUTING. By K.D. Watenpaugh, Physical and Analytical Chemistry, The Upjohn Company, Kalamazoo, MI, USA.

Protein crystallography continues to be a rapidly growing scientific field with new methods and computer software taking advantage of the advances in computer hardware and diffraction equipment. Development of ever more powerful workstations, many with high-performance 3-D graphics, supercomputers, high speed data collection systems are affecting the software developments.

Some areas of software developments include the following.
(1) The refinement process is including other forms of information in addition to the diffraction data. Examples are the programs X-PLOR, GROMOS and CEDAR that include molecular mechanic/dynamic calculations along with the diffraction data. Increased use of other structural information through homology-based modeling will be incorporated directly into the refinement process, as well as for model building.
(2) There are new methods of determining, extending and refining phases using maximum entropy methods and direct methods using anomalous scattering data.
3) We continue to find new ways to use computer graphics for both modeling structures and analyzing them.
(4) With the advent of ultra-fast area detectors on synchrotron sources, new hardware and software to process the data must be developed. Complete data sets will be collected in fractions of a second.
(5) More integrated and general systems of crystallographic software are being developed. Data reduction packages such as MADNES and XENGEN and molecular replacement packages such as MERLOT merge numerous routines focused on a particular area. Large integrated systems such as PROTEIN and (MAC)XTAL are continually being expanded. Portable integrated software systems will become more important with the increased speed by which structures will be determined and with the rapidly changing hardware.

These along with other developments or trends will be discussed with illustrations in the presentation.

MS-02.01.05 PLATON, AN INTEGRATED TOOL FOR THE ANALYSIS OF THE RESULTS OF A SINGLE CRYSTAL STRUCTURE DETERMINATION. By A.L. Spek, Lab. voor Kristal- en Structuurchemie, University of Utrecht, 3584 CH Utrecht, Netherlands.

PLATON is a program for the automated generation and analysis of a large variety of derived geometrical data. In addition several tests for the correctness of a crystal structure are carried out. E.g. an extended version of the MISSYM algorithm (Le Page, J. Appl. Cryst., 1987, **20**, 264-269) to test for missed symmetry is implemented. The program can be used also as a tool to locate solvent accessible voids in the structure and for unit cell transformations. Graphics features include NEWMAN plots and automatic ORTEP plots.

The calculations may be invoked with simple key-words (with optional free-format parameters) and are basically of three types: intra-molecular, inter-molecular and coordination. The necessary chemical data such as atomic weights, various atomic radii and chemical type are drawn from internal tables on the basis of the atom name label.

The intra-molecular calculations include the identification and symmetry expansion of isolated molecules, the tabulation of bond distances, bond angles and torsion angles, the search and analysis of planar parts in the structure, the search of rings (up to 24 membered) and puckering analysis (including Cremer and Pople and asymmetry parameters). All quantities are calculated with standard deviations. In addition, the individual anisotropic thermal motion parameters are analyzed, including the Schomaker and Trueblood (Acta Cryst., 1968, **B24**, 63-76) TLS-model, bond distance corrections and the Hirshfeld 'Rigidbond' test (Acta Cryst., 1976, **A32**, 239-244).

The inter-molecular calculation checks for short inter-molecular contacts and will tabulate the geometry for all hydrogen bonds in the structure (including bifurcation and trifurcation) and analyze for 1, 2 or 3-dimensional networks of hydrogen bonded molecules.

The analysis may be completed with the calculation of the coordination sphere (distances and angles) of relevant atoms (with the calculation of the Berry pseudo-rotation parameter in case of five-coordination) or a scan for the shortest metal-metal distances in the structure.

Various parameter input standards are available including SHELX compatibility and cartesian (Angstrom) coordinates. Space group symmetry may be specified either implicitly with the space group name or explicitly with the symmetry operations.

The program is written in Fortran-77 for VAX/VMS or UNIX and supports various graphics standards including Tektronix and HPGL.

MS-02.01.06 THE CRYSTALLOGRAPHIC WORKBENCH. By P.E. Bourne*, P.M. Marquess, and W.A. Hendrickson, Howard Hughes Medical Institute, Department of Biochemistry and Molecular Biophysics, Columbia University, 630 West 168th Street, New York, New York 10032, USA.

As workstations become more prevalent the opportunity exists to improve the way the crystallographer interacts with the computer. In its simplest form this interaction involves multi-tasking using multiple terminal emulations. However, the window management software that controls terminal emulation may also be used to create a more sophisticated application interface containing dialog boxes, pop-up menus, and so on--in short, a Macintosh type interface. The problem with such an interface is that it is time-consuming to code and not easily expandable to support new application programs. We have developed a Workbench Control Language (WCL) and corresponding interpreter to simplify the design and utilization of sophisticated windowing interfaces for use in scientific programming. Incorporation of an application into a workbench requires no modification to the application Fortran programs. The workbench does, however, impose a file naming convention and a directory organization for all data files.

The Crystallographic Workbench (CW) for protein crystallography is the first application for WCL. CW displays a window hierarchy for the structure under study. The parent or master window contains unit cell and symmetry information which is automatically passed to each program in the appropriate format. Selecting an application opens a child window--a dialog box from which files are selected and optionally edited. One possible file selection opens the input data file window. The format of this window depends on the format of the file: input under keyword style