18.X-5 COMPUTER GRAPHICS IN THE SYNTHESIS, ANALYSIS, AND COMMUNICATION OF BIOMOLECULAR STRUCTURAL INFORMATION. By A.J. Olson, Ph.D., Department of Molecular Biology, Research Institute of Scripps Clinic, U.S.A.

Computer graphics has evolved into the principal modeling tool in biomolecular structural studies. It is used extensively in molecular modeling building, evaluation, and presentation. Hardware and software now exist that enable these activities over a wide range of cost and performance, from personal computers to supercomputer class devices. This paper will review the current application of computer graphics to biomolecular modeling, focusing on the special requirements of each of the principal modeling functions: synthesis, analysis, and communications. Emphasis will be given to developing technologies and high-end performance.

In the hardware arena, new classes of machines have recently appeared that will have significant impact on molecular graphics. The evolutionary growth of the scientific workstation is now at the stage where machines with near supercomputer power and integrated high performance graphics will soon become available. Workstations from Dana Corporation and Stellar are of this class. A new class of machine, the application accelerator will produce similar performance by attaching to existing workstations. The recently announced TACC-1 from Transcept Computer is an example of this type of hardware. Finally, special purpose graphics engines using highly parallel computation are currently prototyped to out-perform all existing display systems. The Pixal Planes machine from the University of North Carolina, will be discussed as an example of this trend.

Software seems to be the major bottleneck in current molecular graphics. We are in a period of transistion from home-built systems to team-built commercial systems. The problem in the near term will be the flexible incorporation of new algorithms from the molecular modeling community into a widely distributed package. Discussion will also touch upon the status of graphics standards and new tools for constructing user interfaces.

The application of computer graphics problems in biomolecular structure will be illustrated by work from the author's laboratory. An example of synthesis activity will be given by discussing the modeling of a novel DNA intercalation mechanism. Analysis activity will be illustrated with the examination of protein-protein interfaces in macromolecular assemblies such as antibody structures and viral capsids. Calculation and representation of a variety of molecular properties including shape, accessibility, electrostatics and mobility are central to this activity. Molecular graphics communication will be illustrated by the presentation of animated sequences on enzyme and viral function.

18.1-1 ENDIX - A COMPUTER PROGRAM TO SIMULATE ENERGY DISPERSIVE X-RAY AND SYNCHROTRON POWDER DIFFRACTION DIAGRAMS. By E. Hovestreydt[1,2], E. Parthé[1] and U. Benedict[3]. [1]Lab. de Cristallographie, Université de Genève, 24 quai E. Ansermet, 1211 Geneva 4, Switzerland. [2]Inst. f. Kristallographie, Universität, Kaiserstr. 12, 7500 Karlsruhe, [3]Europäisches Inst. f. Transurane, Postfach 2266, 7500 Karlsruhe, Federal Republic of Germany.

A FORTRAN computer program is described which allows to simulate energy dispersive X-ray and synchrotron powder diffraction diagrams. The input consists of structural data (space group, unit-cell dimensions, atomic parameters) and information on the experimental conditions (fixed Bragg angle, type of X-ray tube and applied voltage or operating power of synchrotron radiation source). The output consists of a list of normalized intensities of the diffraction lines ordered with increasing energy (keV) and optionally also of an intensity-energy plot. The intensities are calculated with due consideration of the wave-length dependence of both the anomalous dispersion and the absorption coefficients. For a better agreement between the observed and the calculated spectra a provision is made to superimpose optionally on the calculated diffraction line spectrum all additionally observed lines such as e.g. fluorescence- and emission lines as well as escape peaks. The different effects which have been considered in the simulation are discussed to some detail. The program is demonstrated with a calculation of the energy dispersive powder diffraction pattern of UPt_3 with Ni_3Sn structure type.

18.1-2 MISSYM, A PROGRAM FOR THE DERIVATION OF THE SYMMETRY ELEMENTS IMPLIED IN A STRUCTURE DESCRIPTION. By Y. Le Page, Chemistry Division, National Research Council of Canada, Ottawa, Canada, K1A 0R9.

The space-group symmetry implied in the atomic coordinates of a structure can be reconstructed by deriving the metric symmetry elements of the lattice from the cell data, and then finding the location and the intrinsic translation for corresponding space-group symmetry elements with the same orientation using the list of atomic coordinates.

The MISSYM computer program designed along these principles discloses one symmetry element with high multiplicity along each symmetry direction, as well as the inversion center if the structure is centrosymmetric, and the non-lattice-type translations if any is present. The printout lists the indices of the row along which symmetry occurs, followed by the plain English name for the kind of element, coordinates for one point on the element, and the components of its intrinsic translation part. Any trivial item in the output list is omitted, e.g. no glide part is printed for a mirror plane etc. The search order is selected in such a way that the elements printed are often those in the space-group symbol.

MISSYM has correctly treated the known examples of overlooked symmetry or quasi-symmetry on which it was tested. As no computer program operating on refined atomic coordinates can prove the presence of extra symmetry in the crystal, the user should scrutinize the experimental evidence and report either a different space group or the existence of pseudo symmetry whenever extra structural symmetry elements are disclosed by the program. MISSYM is part of the NRCVAX system (Gabe, Lee and Le Page, in Crystallographic Computing 3, Clarendon Press, Oxford pp.167-174 (1985)) which now runs on several virtual memory machines with FORTRAN77 compiler and ASCII internal representation.

To get a copy of NRCVAX and manual, send a 2400 ft magnetic tape to: Dr E.J. Gabe, Chemistry Div., N.R.C., Ottawa, Canada, K1A 0R9. For 1987, and possibly subject to change, there is no charge.