

18.5-02 BILDER: AN INTERACTIVE GRAPHICS PROGRAM FOR BIOPOLYMERS. By R. Diamond, Medical Research Council, Laboratory of Molecular Biology, Hills Road, Cambridge, CB2 2QH, England.

Bilder is an inter-active computer-graphics program developed for an Evans and Sutherland Picture System 1 on a DEC PDP11/50 computer. It is designed to manipulate polymeric structures in relation to an electron density or other map. It can develop a structure *ab-initio* given the sequence or it can make modifications to pre-existing structure, including changes of sequence. It works on a segment of chain of limited length with the remainder of the structure held in spools on disc. Any part(s) of the structure not in the working segment may be made visible and the selection of atoms for this purpose may be based on position in space or position in sequence or atom type or any mix of these criteria. Each end of the working segment is recognised as free or fixed if the associated spool is empty or not empty and this is used to preserve chain continuity. Addition or removal of residues may only be done at a free end. The chain may be severed to create a free end and re-united later, or it may be manipulated under the sustained constraint of chain continuity. Manipulation may be done by associating up to three bonds at a time with continuously variable inputs through a tablet so that possible variations to the structure may be sought and observed. These may then be adopted or not adopted as alterations to the structure. Alternatively, manipulation may be done using a least-squares type of optimizer which responds both to targeted positions for atoms and to target values for conformational angles with assignable weights in both cases. Data for the optimizer is treated as belonging to any of four hierarchies. The first hierarchy consists only of target positions for a small number of atoms required to maintain chain continuity at the interface with each spool (and any other constraints that may be set). Optimization of the conformation against these data normally leads to a rank-deficient normal matrix. Optimization then takes place within the subspace which is determinate, information about the uncommitted degrees of freedom being passed to the next hierarchy in the form of *ortho*-normal vectors. Thus each hierarchy operates within the constraints imposed by all previous hierarchies. As already mentioned, the first hierarchy is used to ensure chain continuity. All other positional targeting information enters the third hierarchy. Target values for angular variables may then be placed in either the second, third or fourth hierarchies. If they enter the second they determine shape in preference to targeted positions. If they enter the third they compete with positional data in a least-squares sense. If they enter the fourth they serve only as defaults in the event that the positional information supplied fails to determine the conformation in respect of such angles. This appears to work successfully and has been accomplished without the overhead of determining eigenvalues and eigenvectors.

The electron density map is pre-contoured and stored as vectors. The volume of the map is divided into bricks of equal volume and the contents of each brick are further divided into elements. Typically, an element consists of contours at a single level on one set of planes. Up to twenty elements are permitted, the brick-element being the smallest quantum of map which may be independently controlled at display time. Maps may be mixed so that X-ray maps, neutron maps, difference maps etc. may be made available simultaneously and displayed together or separately with the same or different line styles. The system has been operational since June 1977.

Diamond R. - In Biomolecular Structure, Conformation, Function and Evolution. R. Srinivasan Ed. (1980), Pergamon Press, Oxford and New York.

18.5-03 CRYSTALLOGRAPHIC USES OF THE SRC MICROFILM RECORDER. By K. M. Crennell, Rutherford & Appleton Laboratories, Chilton, Didcot, Oxon, England.

The SRC microfilm recorder has several cameras and a colour option which allows direct production of colour film for slides or to simulate rotating molecules. It is also used to make camera ready copy for pages of the annual bibliography published by the Cambridge Crystallographic Data Centre. The problems associated with this, with any additional index of chemical structure diagrams, and with general mathematical text will be discussed. Other uses include diagrams made by PLUTO78, and computer simulations of crystal structure defects and electron microscope images. Examples of all of these will be presented and further uses suggested.