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The program CHAIN is the result of our laboratory's long experience in the use of molecular graphics for fitting atomic models to electron density. The program is used to display atomic coordinates and electron density maps on a graphics system and then fits the atomic model to the electron density.

The user first prepares data files containing the desired coordinate and density information. CHAIN then allows one to display up to eight different electron density contour levels, superimposed with atomic coordinates on the screen. One can then interactively modify the coordinates.

A number of additional features are included with the program; they initiate various routines to automatically regularize or refine the coordinates and to display them in a variety of ways. The program also provides a number of interfaces to read in and write out the atomic coordinate information so it can use data from and be used by non-CHAIN programs.

CHAIN is actually a series of tightly and logically coupled subroutines connected via a main parser. As keyword commands are given to the program, the parser interprets the command and invokes the required subprogram to perform the desired function. Because of this type of organization, new subprograms can be added easily to CHAIN, provided that they are able to uiltize the CHAIN file formats. Additional entries can be added to the keyword list along with the appropriate calling routines.

The program also contains an on-line utility to allow the user to obtain immediate assistance with any command. A 200-page manual accompanies the distribution.

The program is designed, at present, to run on an Evans & Sutherland PS300 graphics unit.

Chemical Graphics Input/Output Package for the Cambridge Structural Database

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The Cambridge Structural Database (CSD) is the world's leading database of molecular structure. It is a unique collection of chemical, numeric and bibliographic information for all published organocarbon compounds analyzed by X-ray or neutron diffraction. It is thus an invaluable tool in computer-aided drug design and in the analysis of geometrical parameters to obtain new insights into structure and bonding.

A core program, QUEST88, lets users search bibliographic, chemical connectivity and selected numerical data within a single query. Tests of individual fields are combined via logical operators to form a complete question.

A graphical input/output package has now been developed for inclusion in QUEST89, which will replace the current alphanumeric coding of the search question. Queries may be input via a fully interactive, menu-driven interface. Substructure, textual and numeric searches may all be specified from within this integrated package.

Six menus provide the ability to generate a substructure, which may be edited, saved for future use or combined with further bibliographic or numerical questions using the logical operators AND, OR and NOT. The complete query is then passed to the database search software.

Special features of the input package include

- over 60 system templates, including hydrocarbons, steroids, and porphyrins
- the ability to save and reread user-defined templates
- Feldmann ring notation: e.g., 66U6D5 specifies the steroid skeleton
- full UNDO facility, with journaling, to rerun a previous session
- a powerful editing facility, for generating production-quality chemical diagrams
- symmetry operations, and a "copy" facility, which may be applied to complete structures of fragments, for efficient generation of high-quality diagrams
- a full on-line HELP facility

Output from QUEST88 is enhanced by the generation of two-dimensional (2D) chemical diagrams. These publication-quality diagrams use x,y atomic coordinates, generated via CCDC in-house software, which are now incorporated within the chemical connectivity records. They will form part of future database releases. Substructures located by QUEST88 can be highlighted on these diagrams. 3D crystallographic (molecular) diagrams can also be selected for the display of hits.

The interface program, like QUEST88, is written in standard FORTRAN77 and sends Tektronix escape codes to the terminal. Tektronix 4010/4014 (monochrome), 4100 Series (color) and 4200 Series (color) terminals and emulators are supported. For the 4010/4014 and 4105 standards, software emulation of the 4200-style "dialog area" facility is provided.

Menu operation is controlled by a graphical input (GIN) device, such as a mouse or tablet, or simply via cursor keys. At all times, however, the menus may be suppressed by typing commands manually, thus providing greater flexibility for experienced users. (The Tektronix 4200F4M three-button mouse and Tektronix 4957 tablet are supported, although the program requires only a one-button device for operation.) In addition, HP–GL plotters are supported, for generating hard copy.

The complete graphical input/output system has been developed to provide easier access to CSD's already extremely powerful search software. It will be released to academic and industrial users in 1989.