Computer Hardware

The CAD 4 is available in numerous configurations based upon the user's requirements.

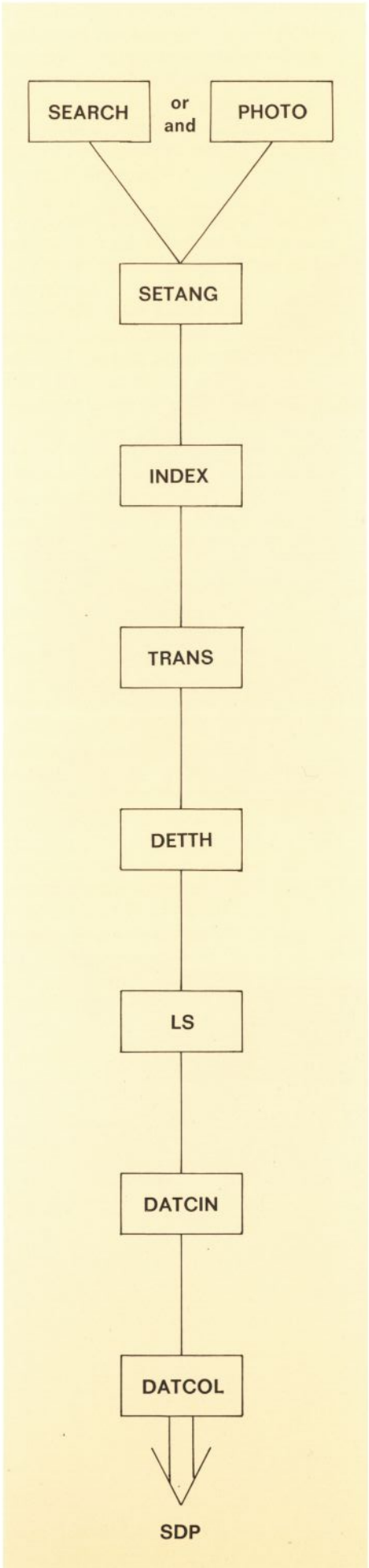
The basic CAD 4 configuration uses the Digital Equipment PDP-8 computer with a 8K core memory together with a movable head disk RK 8. The disk is used to store the programs and the experimental results temporarily. Once read to the disk, all necessary diffractometer programs and mathematical programs remain in the system and can always be used without requiring any special loading.

A highly efficient operator system to communicate via terminal with the computer and to work optimally with the disk is provided with the instrument. The system enables the user to run long programs with a small computer core memory. There is ample space for program extensions.

For systems utilizing an expanded PDP-8 with 16K core memory (CAD 4 F), the programs are supplied in FORTRAN IV. If a PDP-11/34 or PDP-11/60 system is selected for diffractometer control (CAD 4 SDP) FORTRAN IV programs are also used. Then the programs are working in dynamical priority time-sharing mode. If 32K of core memory, floating point hardware, two 1.2 million words disks (or other mass storage disk) and magnetic tape are included, then structure calculating programs are supplied as part of the Enraf Nonius Crystallographic System ENX.
The interface between diffractometer and computer is designed with standard I.C. logic modules, assuring easy interchangeability. The CAD 4 system includes a high efficiency magnetic tape recorder. A synchronous IBM-compatible write/read recorder makes condensed storage of the measuring results possible. Either 7- or 9-track available. Configuration with DEC tape on request. Produced tapes are immediately usable on computers without any conversion, greatly improving data processing.

Standard terminal is the DECwriter. Other terminals are available.

Whilst the software for diffractometer control is equally comprehensive and complete for all versions of the CAD 4 and whilst the operations are the same for CAD 4, CAD 4 F and CAD 4 SDP the language is different. Programs for the basic CAD 4 are written in Assembler, whereas program language for CAD 4 F and CAD 4 SDP is FORTRAN IV.



Condensed CAD 4 Software Description

The 'CAD 4 SYSTEM' is a disk oriented operator system. It is composed of various main programs, subroutines and space for storing required variables. Programs or data are swapped by program from the disk to the core memory. It gives instructions to the operator via terminal or accepts instructions from the operator in a convenient and simple interactive manner. The open structure of the system facilitates changes and the addition of programs to suit particular requirements.

Automatic reflection search program

- works without any input about the crystal to be investigated
- starts with the only optically centered crystal
- leaves the user free to choose the 2θ starting value
- can work on fixed 2θ value if desired, e.g. to find specific reflection
- automatically looks for 25 reflections
- optimizes automatically these reflection positions in 3 angles ω, 2θ, κ
- determines necessary scan width for all reflections found
- determines integrated net intensities of all reflections found
- determines peak position and gravity center of each reflection
- outputs scan profile on terminal on command
- stores a list of the optimized reflection positions with all included information and outputs on request.

Reflection search program using film coordinates input

- starting inputs are the film coordinates of reflections on a rotating crystal Polaroid photograph made on the diffractometer
- calculates automatically correct ω, 2θ and κ values
  looks for correct φ value
- optimizes automatically these reflection positions in 3 angles ω, 2θ, κ
- determines necessary scan width for all reflections found
- determines integrated net intensities of all reflections found
- determines peak position and gravity center of each reflection
- outputs scan profile on DECwriter on command
- stores a list of the optimized reflection positions with all included information and outputs it.