

CAD 4 SDP

The growing concern about the cost of crystallographic computing has encouraged crystallographers to look for alternative ways of performing their calculations. With the advent of relatively inexpensive small computers, capable of rapid execution times and readily accessible disk storage, it became clear that a powerful new crystallographic tool was potentially available. The need for an integrated library of crystallographic programs designed for a small computer was apparent.

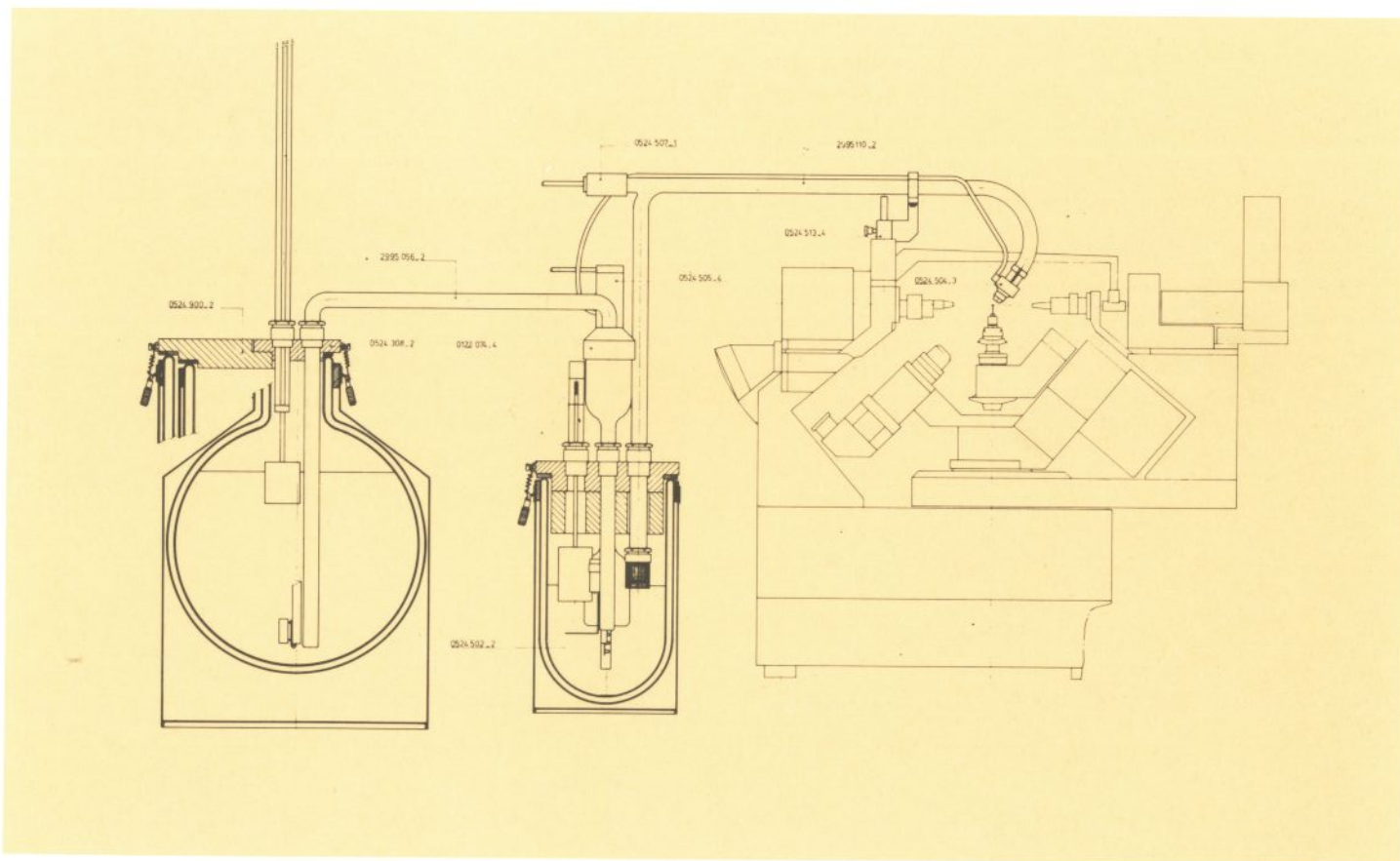
The Enraf Nonius **structure determination package** (SDP) is such an integrated set of remarkably fast

programs, developed for use on the PDP-11 series of computers. The complete Enraf Nonius structure determination system CAD 4 SDP consists of the standard X-ray generator, Kappa-axis-goniometer hardware and counting chain hooked up to a PDP 11/34 or PDP 11/60 computer system. The computer hardware includes a minimum of 32K core memory, floating point hardware, two moveable head disk systems, IBM compatible tape drive, line printer/plotter and one or more terminals. CAD 4 diffractometer and structure calculations SDP are run simultaneously in a time share mode program.

Language for both diffractometer control and structure calculations is Fortran IV with the exception of a few assembler language subroutines. The SDP programs compile, link, and execute in 32K of core and take advantage of rapid access to a moving head disk for storage of large arrays.

The package includes programs for data reduction, direct methods phase determination, Fourier calculations, least-squares refinement, function and error calculations, plot and table productions, etc. For more detailed information is referred to the CAD 4 SDP leaflet.

Low temperature work



The Enraf Nonius Universal Low Temperature Device, FR 524H, uses liquid nitrogen cooling for temperatures down to approximately -170°C . It does not limit the accessible diffraction sphere and the movements of the goniometer in any way.

Permanent improvements of this accessory achieved in close

co-operation with the Institute for Structure Chemistry of the University of Groningen have led to an easily operable system with good temperature stability and a low temperature gradient at the crystal position.

A cryostat to work at temperatures down to approximately 10°K has been developed for use with the CAD 4. This cryostat, CT 73, uses liquid helium. Whilst there is some obscuration caused by the device, it leaves great directional freedom under these extreme circumstances. For more detailed information read the specific literature.