

NOTICE DE PRÉSENTATION DU DIFFRACTOMÈTRE QUATRE CERCLES CAD4 ENRAF-NONIUS

FICHE N° 3997

PRÉSERVER
SAUVEGARDER
VALORISER

Période de fabrication : 1950-1974

Fabricant : ENRAF-NONIUS

Domaines : Chimie, Physique

Sous-domaines : Cristallographie, Chimie inorganique, Chimie du solide, Cristallographie, Physique

Organisme : Université de Rennes

Ville : Rennes

Modèle : CAD 4 Kappa Axis

Matériaux : Papier

Description

Ce manuel de présentation en anglais a été édité par la société Enraf-Nonius pour présenter le diffractomètre quatre cercles Cad4 Kappa. En une dizaine de pages, elle présente l'appareil, ses caractéristiques et périphériques, les programmes de calcul et le travail en basse température.

Utilisation

Ce manuel présente le diffractomètre Cad4. Il était utilisé par les chercheurs de physique et de chimie de l'université de Rennes dans le cadre d'un service commun de radiocristallographie rattaché au laboratoire de cristalochimie de Rennes (Directeur : Daniel Grandjean). Ce diffractomètre a servi à l'enregistrement d'intensités diffractées par des monocristaux. A partir de ces données de rayons X, les chercheurs modélisaient et déterminaient la structure atomique des matériaux étudiés. Ces mesures traitées par ordinateur permettent par transformée de Fourier de reconstituer l'image du cristal et surtout de la molécule de base qui le compose.



A microscope, which gives a comfortable 60 x magnification and has a graduated reticule, is fixed to the omega bracket. This microscope remains aligned during the operation of the diffractometer and does not give any obscuration or physical interference.

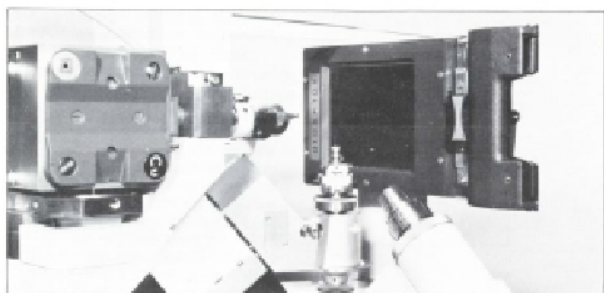
It is placed to enable the user of the diffractometer to make the necessary primary centering adjustments of the crystal.

A second microscope which can be mounted independently of any movement of the goniometer is supplied as an extra optional.

A highly stable eucentric goniometer head with a test crystal mounted is provided as standard with the diffractometer.

All axes, the attenuation filter, the aperture disk, etc., can be controlled with a portable control unit which has in detail the following functions:

- key operated main switch for manual or computer operation of the goniometer
- shutter switch and pilot lamp
- balanced filter switch
- attenuation filter switch
- motor direction switch
- speed range selector
- motor speed continuous variation button
- motor selector for phi, kappa, omega, 2 theta and aperture disk
- collision switch override buttons.



Polaroid Cassette

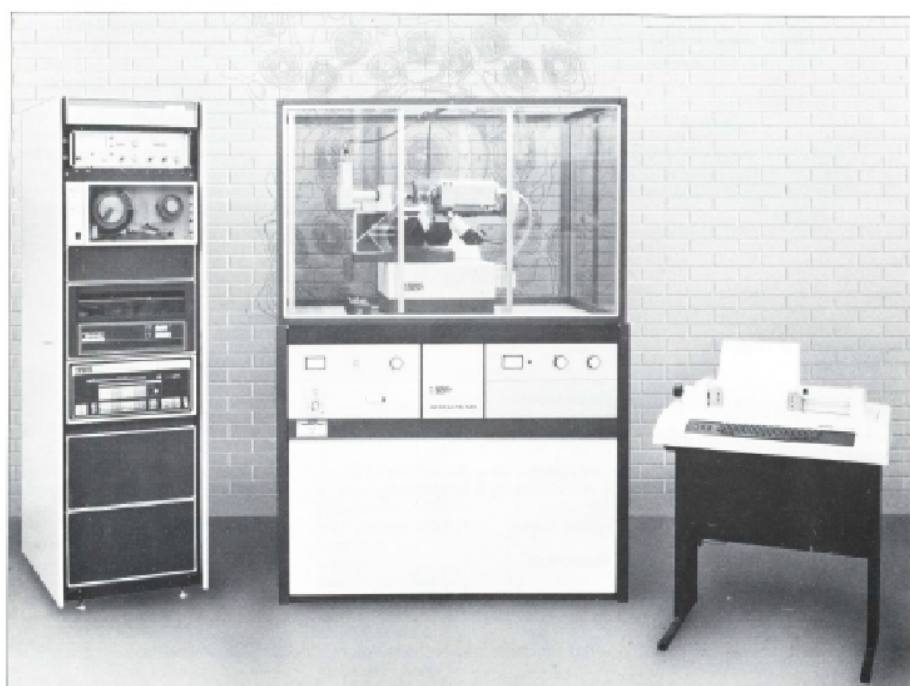
A Polaroid XR 57/1 cassette can be attached to the goniometer base allowing Laue- or rotating crystal exposures; rotating crystal exposures can be used to calculate a first reciprocal axis matrix of a non-aligned crystal. This provides one alternative to start with a not aligned and possibly unknown crystal. (The other alternative is the very efficient automatic reflection search). The Polaroid exposure will give interesting information about crystal quality and symmetry.

Environmental Enclosure

The new Enraf Nonius environmental enclosure provides maximum safety for the user and at the same time optimum access to the goniometer. The enclosure can be opened from any side. The doors are provided with interlocks closing the X-ray port if one door should be opened during operation.

**Main characteristics of the
CAD 4 Kappa
Diffractometer**

- an absolute minimum of physical obscuring and interferences
- optimal ranges for all angular movements
- full omega rotation without mechanical interferences
- optimal range of reciprocal space can be reached
- azimuth rotation possible for each reflection
- great accessibility of the crystal for all types of accessories
- a most accurate construction due to a bearing mounted axis instead of the arc cradle principle
- optimal long-life accuracy
- easily changed crystal-detector distance
- easy and quick tube alignment with the use of program
- balanced filter unit
- graphite monochromator included in standard package
- continuously variable and program controlled detector aperture
- absolute encoders on all axes and on detector aperture
- 8K or 16K computer with 1.6 Mwords disk standard
- IBM compatible magnetic tape recorder
- most reliable, fast and quiet DECwriter standard terminal
- disk-operating system with very versatile operator's program offers maximum disk utilization and simplified program changes
- most versatile and automatic software
- Polaroid cassette for Leue - or rotating crystal exposures is easily attachable
- low temperature liquid nitrogen or helium systems available
- complete manual control possible, by portable control unit.





CAD 4 Kappa Axis Diffractometers

CAD 4

CAD4F

CAD 4 SDP

More than 50 years experience in x-ray diffraction

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.

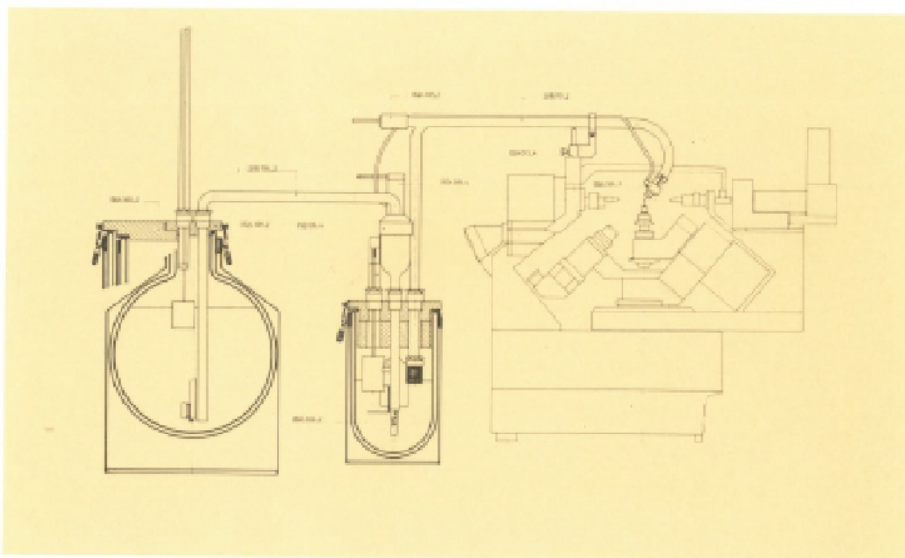
The Enraf Nonius structure determination package (SDP) is such an integrated set of remarkably fast

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 crystal 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.



Pour nous citer :

Base de la Mission nationale de sauvegarde et de valorisation du patrimoine scientifique et technique contemporain, PATSTEC, Notice de présentation du diffractomètre quatre cercles Cad4 Enraf-Nonius (ENRAF-NONIUS), <https://www.patstec.fr/ressources/objets/detail?id=16015>, consulté le 2026-10-23