

- calculate orientation matrix using a list of at least three reflections
- need no further input if the list formed after optimization or indexing will be used
- do least-squares refinement
- determine accurate unit cell parameters
- determine standard deviation of unit cell parameters and matrix components
- calculate h k l limits
- calculate the vector components
- do all calculations in relation to orientation matrix and goniometer position such as change of azimuth position and recalculation of bisecting position
- correct on command reflection positions automatically in case of focus missettings or optical miscentering of the crystal.

Automatic data collection program

- provides different scan possibilities such as ω , $\theta/2\theta$, and various. ω/θ scan modes which enables user to reduce aperture width to improve peak/background ratios
- does automatic datacollection at various azimuth angles (rotation around diffraction vector) for empirical absorption correction or multiple reflection test
- provides fixed or variable (program control) scan during operation
- uses variable scan angle and receiving aperture width depending on θ ($K\alpha_1/K\alpha_2$ separation)
- generates h k l in a selectable ZIGZAG pattern;
- accepts manual h k l input or prepared list of h k l's
- skips automatically systematic extinctions
- provides the possibility of Friedel measurements
- provides automatic balanced filter measurements
- does intensity measurement using a continuous scan of 96 single measurements
- stores either: background/intensity/background or complete reflection profile on disk on simple command
- prints short or extended information depending on switch position
- copies short or extended information to tape or other I/O device, including X-ray exposure time
- outputs to terminal only special data like intensity monitors on request

- provides up to 25 control reflections for intensity monitoring; desired intensity and limits of absolute variation are input values
- measures control reflection after a pre-selected time of X-ray exposure as defined in input
- provides program controlled sequence of data collection,
- reoptimization and recalculation of orientation matrix
- provides angular stability control using up to 25 control reflections
- reoptimization and recalculation of orientation matrix using up to 25 control reflections
- measures all reflections with statistical accuracy defined in input
- calculates scan speed for slow scan after prescan depending on desired accuracy
- skips slow scan depending on given low intensity limit
- does repeated scan, if specified, and integrated intensity measurement, does equality test of the two results
- repeats automatically intensity measurement up to 3 times in case of non-equality
- performs continuous scans around reflections and scans in a certain direction of the reciprocal space
- provides special four circle measuring program to measure intensities at a crystal positioning with minimum absorption loss (important when strongly absorbing materials crystallize in needles or plates)
- modifies in data collection input simply by changing the concerned address or addresses after interruption, automatic continuation of data collection after a simple command
- saves and recalls all input values
- provides data output to terminal, 7 or 9 track magnetic tape or other selected I/O device like papertape puncher if requested
- uses standard magnetic tape code BCD, ASCII, EBCDIC or any other available code
- data blocks written on magnetic tape are checked after writing and rewritten if wrong; all blocks are written twice
- calls for operator in case high voltage is off, magnetic tape at end or similar situations.

General operator program

- does calculations from Eulerian geometry to Kappa geometry and vice versa

- replaces manual operation with the diffractometer by terminal commands such as
 - positioning to angles given in Kappa or Eulerian geometry
 - positioning to h k l
 - positioning to different azimuth angle
 - positioning to negative 2θ value
 - positioning to Friedel - correspondent reflection
 - display of precise encoder position
 - operation of shutter, aperture, diaphragm and filter
- does ω , 2θ or χ (combination of κ and ω) scan or any other combination scan at a given position using input value for scan angles, scan speed, and aperture width
- displays reflection profile on terminal
- outputs intensity and deviation of peak position and center of gravity.

Loading and saving programs

- program to load disk with software from magnetic tape
- program to save disk contents on magnetic tape
- program to make terminal display of the tape contents.

Diagnostic programs

- program to check operation of magnetic tape
- program to check the interface
- program to check the goniometer function including encoder system, motors, friction, etc.

Data reduction program

- does Lorentz-polarisation correction
- does empirical absorption correction
- works on datacollection output file
- produces new disk file with observed structure factors.

Other programs

The user is supplied with DEC standard programs. The complete package exceeds all software of comparable computer systems. Some of these standard programs are stored on the disk together with Enraf Nonius programs.