The control program for the Enraf-Nonius CAD-4 diffractometer has been enhanced. Although the CAD-4 configuration used in the development of the Enraf-Nonius programmable diffractometer was tested on the DEC FORTRAN-IV compiler (3), similar success has been achieved with DEC's FORTRAN-77 compilers. The current NRCCAD version incorporates all the original Nonius commands plus numerous modifications and additions. The capability to run the diffractometer from a terminal attached to either the host computer or the interface is retained, but the communications code has been modified so that response times at a terminal attached to the host are greatly improved. All dialogue and prompts have been expanded and clarified and a number of checklists have been added. The procedure to start and stop the program has been simplified and the program can now be restarted without reloading the interface programs.

A number of modifications have been made in the interface programs to permit scans with up to 512 steps. The system is distributed with a set of command files that will generate the required tasks after the operator answers a few simple questions. The following facilities have been added. The Nonius reflection centering algorithm, to which the criticism of Frevel et al. (Frel); Le., U.; and Kistemaker J.D., 1983, J. Appl. Cryst. 16, 195-219, has been enhanced to overcome this objection in cases where reflections with little or no overlap can be used. The list of reflections for which overlap or a space group symbol with the correct number of unique axes and vertical or horizontal peak separations in front of the detector, all procedures designed for a Eulerian cradle; for scans over pairs of twin reflections, the coupling factor between and is computed individually; (6) minimal or maximal separation of twin pairs in the equatorial plane of the instrument (K. Tichy); H. Enges, Helv. Phys. Acta, 1977, 50, 459-466; (7) control of reflection overlap in critical situations (Y. Benner et al., J. Appl. Cryst. 1979, 12, 177-179; (8) control of intensity being cut off by the apertures.

Two-dimensional (2D, 2D) intensity distributions are calculated for the case of crystal-monochromated (pyrolytic graphite) X-radiation incident on a small specimen (15). The calculations are based on ray-tracing and take into account the mosaic spread of the monochromator, depth of penetration into the monochromator, source emissivity distribution, wavelength distribution, broadening due to the detector aperture, and various aspects of the experimental arrangement involved. The calculations are compared with experimental results and reveal excellent agreement.

A full understanding of such intensity distributions can yield detailed information about the nature of the individual components present. The analysis can also provide details essential to carrying out conventional one-dimensional (1D) profile measurements in a correct and consistent manner.