**NKET**

This is a complete data set for a small organic structure.

Formula: C8 H13 N O4

Space Group: P 41

Unit Cell: 7.533 7.533 15.780

Z: 4

Cell contents: C32 H52 N4 O16

Radiation: Cu

Reflections: Fsq in HKLF file NKET.REF, FORMAT(3I4,2F8.0)

Size: .2x.2x.7 mm

It will easily solve with SIR, SHELXS or MULTAN.

The primary data from an ENREAF‑NONIUS CAD4 is:

NKET.DAT the reflection data

NKET.PSI the psi profile.

The data can be processed through RC93, to give the files:

NKET.HKL the processed reflection data

NKET.SCF the unit cell, scale factors etc.

NKET.ABS the processed phi scan.

This preprocessed data can be entered into CRYSTALS in SCRIPT mode, when the dialogue ROUTINE should lead you to solve and refine the structure.

The same data can be entered in COMMAND mode, (as USE files) and provides a small but interesting test set for getting acquainted with CRYSTALS facilities.

The file NKET.SLX is the result of a SHELXS run, and can be copied to

SHELXS.CRY if you don't wish to run SHELXS but just use the output.

For users migrating from other systems, the folowing files may be run in the order give as an example of the principal steps.

NKET.QCK Getting the basic data in

NKET.LSQ A bit of refinement

NKET.ANISO Sorting out the non‑C atoms and aniso refinement

NKET.FOUR Looking for hydrogen

NKET.REF HKLF format reflections (Fsq)