16.2–8   DIFFRACTOMETER SOFTWARE (CAD4F).

by J.L. de Boer[x] and A.J.M. Duisenberg[xx]

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The CAD4F/OS8 (FORTRAN IV) software is updated and now
includes as new facilities:
ANIVEC: analyzing and handling of high anisotropic
mosaicity. Also suited for split and most types of
twinned crystals. (1)
BATCH: diffractometer control input is read from a
batch input file, enabling the user to compose a comp-
lete, automatic, job.
CONE SEARCH: looks for a particular reflection, lying
on the surface of a cone, whose axis is given by the
position of one known reflection.
(LOW)_TEMPERATURE CONTROL: computer controlled, accur-
ate temperature setting (range: 85-305K, stability:
$\pm$ 0.2°). Temperature is read and stored with each int-
ensity measurement. Data collection possible at various
pre-chosen temperatures by using BATCH.   (4)
MULREF: avoids multiple reflections by analizing an
azimuthal range for each reflection
OTPLOT: omega/theta plot of a reflection. Facilitates
the choice of scan parameters   (2,3)
Q-MODE: data collection on non commensurate structures,
using a fourth, broken, index.
SET4: setting angles derived from four settings of each
listed reflection, leading to cell dimensions freed
largely from mis-alignment errors.
1) A.J.M. Duisenberg, Acta Cryst.(1983).A39, 211-216
2) CAD4 Manual, ENRAF-NONIUS, Delft(1977). ChXIII,p30
3) A.McL. Mathieson, Acta Cryst.(1982).A38, 378-387
4) J.L. de Boer, K.D. Bronsema and G.A. Wiegers. This
conference.

**16.2–9   CELL PARAMETER REFINEMENTS OF SMALL
            CRYSTALS USING A SINGLE CRYSTAL
SPECTROMETER. By V.I.Lisoivan, S.A.Gromilov,
Institute of Inorganic Chemistry, Siberian
Branch of the Academy of Sciences of the USSR.**

The methods of a samples selection and initial
cell parameter determination of single crys-
tals with unknown structures have already been
described (G.B.Bokij, M.A.Porai-Koshits, X-ray
Anal. vol.1 (1964)). These parameters may be
refined using the single crystal spectrometer
(V.I.Lisoivan, R.R.Dikovskaia, Prib. Tekn.
Eksp. (1969) 4, 162). The sample must be so
mounted that its axis would pass   along the
spectrometer axis. Two linear and one angular
parameter may be refined when the crystallo-
graphic axis directions of the sample are de-
termined. Otherwise, it is necessary to find
some reflections, to plot a reciprocal lattice
net and to choose basal planes. The polar co-
ordinates for the origin point in plotting the
reciprocal lattice are $\jmath^* =0$, $\rho =1/d$. For the
next points $\jmath^*$ angle is determined by:$2(180-\jmath^*)=$
$\varphi_{n1}+\varphi_{n2}-\varphi_{o1}-\varphi_{o2}$, where φ_{n1} and φ_{n2} are the angular
positions of n plane for reflections on both
sides of zero, and φ_{o1} , φ_{o2} are those of the
origin point. The remaining lattice parameters are
refined, when the crystal axis is set in the
equatorial plane of the spectrometer. The ref-
lection angle measurements with the 5" accura-
cy can be carried out by the method described
by R.L.Barns (Adv. X-ray Anal. (1972) 15,330).
The method is illustrated by the example of
the inner complex compound bis-[4-(2-oxisty-
ryl)methyl-2,2,5,5-tetramethyl-3-imidazolin-1-
oxil] cobalt(II): a=12,8943(8)Å, b=19,336(1)Å,
c=12,8236(7)Å, $\beta =110,458(6)°$ (without refrac-
tion correction).

**16.2–10   A NEW TWO-CRYSTAL MONOCHROMATOR FOR
            SYNCHROTRON X-RAYS WITH FAST AND PRE-
CISE SCAN IN THE RANGE 5°$\leq$ $\Theta_{BRAGG}\leq$ 85°.**
By U.Bonse,Th.Risse,R.Nußhardt,U.Dretzler,
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D-4600 Dortmund 50, Fed.Rep. of Germany.

For making best use of the unique properties of
synchrotron X-rays in crystallography it is
essential to have at hand a monochromator
system fulfilling the following requirements:
1. High energy resolution E/$_{\Delta E}$ at good trans-
mission, with the option to decrease E/$_{\Delta E}$ at
the benefit of transmission.   2. Wide tuning
range of typically 5keV$\leq$E$\leq$100keV.   3. Possibi-
lity of either reject or choose a single or a
given set of harmonics.   4. Mechanical/thermal
stability.   5. On-line computer operation with
flexibility to change mode of operation accor-
ding to varying user requirements.   6. Fixed
position of incident and monochromatized beam.

We have built a corresponding device in which
two crystals C_1 and C_2 are translated in
opposite direction by a pair of coupled lead
screws combined with precision sleds. Trough-
out the motion paralellism of C_1 and C_2 is
maintained by means of a pair of parallel
guides operating at right angles with respect
to each other similar to the device of
Golovchenko, Leversque and Cowan (Rev.Sci.
Instr.52,509(1981)). The accessible range for
the Bragg angle Θ_B is 5°$\leq$ Θ_B $\leq$85°. The resolu-
tion for the translation is 0.5 μm per step
and encoder unit. This ensures even in the low
Bragg angle range an energy increment
$\Delta E\leq$0.1eV. Fine alignment of the crystals with
respect to parallelism is achieved by combined
stepping motor piezo-electric drives at
crystals C_1 and C_2. This fine control also
alows the rejection/selection of harmonics
by means of suitable misalignment with respect
to exact parallelorientation.

The instrument is operable through a micro-
computer. First results obtained at DORIS/
HASYLAB will be presented.

Fig. 1: Beam paths for three different
       Bragg angles Θ_B

       C_1 C_2: Θ_B = 5°
       C_1' C_2': Θ_B = 45°
       C_1'' C_2'': Θ_B = 85°