N-TREOR Manual

N-TREOR

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C
C This is a Stand-alone version of N-TREOR (Version April 2000).
C
C REFERENCE:
C New techniques for indexing: N-TREOR in EXPO
C (to be published in) Journal of Applied Crystallography
C by Angela Altomare, Carmelo Giacovazzo, Antonietta Guagliardi,
C Anna Grazia Giuseppina Moliterni, Rosanna Rizzi and Per-Erik
C Werner
C
C In EXPO N-TREOR is combined with a peak search procedure and a
C a program set for structure determination.
C
C If you are only interested in the description of how to run the
C stand-alone version of the program go to the headline:
C STREOR the stand-alone version of N-TREOR
C
C N-TREOR (Version April 2000).
C N-TREOR is an updated version of TREOR90 described below.
C The main changes characterizing N-TREOR with respect to TREOR90
C are:
C 1) Several decisions normally made by the user of TREOR90 when
C a default run fails or when a plausible solution is found
C are automatically made by N-TREOR
C a) If a plausible solution is found, the program will look for
C a better solution in a new trial. This may be achieved by
C requiring a higher M20 value or all the first 20 peaks to be
C indexed.
C b) If N-TREOR does not give satisfactory results in a default
C run it repeats the unit cell search with wider error limits.
C c) If still no solution is found, with increased error limits,
C the maximum (h,k,l) Miller indices of the orthorhombic and
C monoclinic base lines are increased and the error limits are
C narrowed to 50 per cent of the default values. ( The reason
C for narrowing the error limits is that a large number of big
C erroneous unit cells may otherwise be generated in the trial
C phase, and correct solutions may be eliminated before
C refinement. There is always a need for more accurate data if
C the unit cell is big. The figure-of-merit tests will
C otherwise fail.)
C 2) The maximum cell volume and the maximum axis values
C investigated by N-TREOR are preset to 4000 A**3 and 35 A,
C respectively, if the maximum observed d value is greater
C than 10 A. If the maximum observed d value is less than 10 A
C the default values are (as shown in the key-word list below)
C 2000 A**3 and 25 A, respectively.
C 3) The dominant-zone tests in TREOR90 are improved, and if more
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C than the first 6 peaks can be indexed by a two-dimensional
C rectangular cell,but no three-dimensional solution is found,
C the first non-indexed peak is reported as a possible
C impurity line that may be deleted in a second test.
C 4) Wavelength dependence of D1 and D2 (error tolerances, see
C the key-word list below) has been introduced.
C DX = DXCU*(WAVE/1.560598)**2 where
C DXCU = D1 and D2, respectively for CuK-alpha1 radiation
C 5) Monoclinic solutions are checked for possible rhombohedral
C symmetry. If the symmetry is likely to be rhombohedral,
C N-TREOR calculates the possible hexagonal axes. In general,
C however, the user has to check for geometrical ambiguities.
C 6) Possible zero shifts in the 2theta Bragg angles are tested.
C This is probably the most serious systematic error in powder
C diffractometry. Although well known internal as well as
C external standard techniques exist, that can be used to
C completely (or almost completely) eliminate such errors, the
C experience from a large number of indexing problems shows
C that zero point errors are frequently present in data sets
C used for powder indexing. (Suprisingly enough even modern
C synchrotron data, with exceptionally high RELATIVE accuracy,
C have sometimes been found to have large zero point errors.)
C 7) N-TREOR can suggest more candidate cells. In order to select
C the best one, a modified de Wolff figure of merit M'20 has
C been introduced, with
C M'20 = (7-N-par)*M20 where
C N-par is the number of cell parameters to be determined (6
C for triclinic system, 4 for monoclinic,....), and M20 is the
C original de Wolff figure of merit. Even if M20 is effective
C as a tool for assessing the reliability of the cell, the
C heuristic relation (M'20=.....) allows the program to prefer
C a higher symmetry solution. E.g., of two possible unit cells
C with similar M20 values, one monoclinic and the other
C triclinic, the monoclinic is preferred by M'20.
C 8) The program PIRUM, originally an interactive program, has
C been suitably modified in order to automatically refine the
C unit cell parameters, without any user intervention. N-TREOR
C performs a statistical study of index parity of the assigned
C reflections in order to detect the presence of doubled axes
C or of additional lattice points (A, B, C, I, R or F centered
C cell). In these cases the reflection conditions are suitably
C modified and the unit cell parameters are again refined.
C Additional refinement cycles are performed by PIRUM after
C applying two supplementary origin shifts of +- one quarter
C of the shift value selected by N-TREOR according to point 6
C above.
C 9) It is not possible to interrupt the calculations by pressing
C the key...I....This option is not available any more.
C 10) It is still possible to use the key-word system as described
C below. Normally, however, only WAVE, LIMIT, CHOICE and END*

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C are needed.
C
C
C STREOR the stand-alone version of N-TREOR
C
C Data input file:
C
C LINE ONE. TITLE Any text in col.2-80
C
C
C LINE SET TWO. One d-value and optionally INTENSITY on each
C line. (Free format)
C It is also possible to use other types of
C input data. See keyword CHOICE in the key-
C word list below. Note that the default value
C of CHOICE is 4 in STREOR (i.e. d-values).
C The data must be given in order, starting
C with the low order lines.Generally the first
C 20-25 lines should be used. Remaining lines
C (if any) may be used in later final refine-
C ments. (The dialogue version of PIRUM).
C
C INTENSITY data is optional. It is never used
C by the program. If present, it will only be
C transferred to the output lists as (max.) 4
C digits integers.
C
C
C STOP LINE FOR LINE SET TWO IS A BLANK LINE
C
C The program will ask for file names and Theta-shift.
C The normal Theta-shift is the step used in the data collection;
C (Usually =0.01) i.e. 0.02 deg. in 2theta.
C
C
C LINE SET THREE.(See general description of this line set below)
C
C Below 4 examples of line set three for STREOR are given:
C
C Example 1.
C end*
C Comment:This is the only key-word needed for a normal STREOR run
C if CuK-alpha1 radiation has been used and d-values are given.
C
C Example 2.
C wave=1.529, end*
C Comment: Error limits are wave-length dependent. It is therefore
C important to give the wave-lenght, although the d-values are not
C wave-lenght dependent. Do not forget the , before next key-word.
C
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C Example 3.
C limit=1, end*
C Comment: LIMIT is a new key-word, not present earlier in TREOR.
C LIMIT can be any integer between 1 and 10 (default value is 10).
C The parameter LIMIT can be given a value less than 10 in order
C to reduce the maximum number of zero shifts tested. ( The number
C of zero shifts applied will be dependent on the result of the
C the calculations and therefore usually less than 10).
C If you have good reason to belive that the zero point error is
C negligible, you may save a lot of computer time by limit=1
C
C Example 4.
C choice=0, limit=1, end*
C Comment: Input data are sine square theta values derived from
C an instrument with strictly monochromatic CuK-alpha1 radiation.
C About limit=1, see example 3 above.
C
C WARNINGS:
C A) In the present version of the program the automatic tests of
C index parity are NOT complete. See comments about VISUAL
C INSPECTION in the condensed output list. ( May be improved in a
C later program version.)
C B) On a PC the calculations may be very time consuming. It can
C be recommended to use LIMIT=1 ( see Example 3 above) in a first
C test run, at least if you have good reason to believe that the
C zero point error is negligible.
C
C
C END OF INSTRUCTIONS FOR THE STAND-ALONE VERSION STREOR OF N-
TREOR
C
C
C
C TTTTTTT RRRR EEEEEE OOOOO RRRR 9999 0000
C T R R E O O R R 9 9 0 0
C T R R E O O R R 9 9 0 0
C T RRRR EEEEEE O O RRRR 99999 0 0
C T R R E O O R R 9 0 0
C T R R E O O R R 9 0 0
C T R R EEEEEE OOOOO R R 9 0000
C
C This is an autoindexing program and should be used to find a
C physically plausible solution to an indexing problem.
C It is not a program for final refinement of the unit cell
C dimensions. (c.f. PIRUM or NBS*AIDS83)
C
C Information for the programmer:
C
C The TREOR99 version is written in Microsoft Fortran for PC.
C
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C The interrupt function (..press the letter i) is generally
C not needed and if you want to use other compilers and/or
C computers whithout any possibility to sense keyboard oper-
C ations during the calculations, you may skip this in the
C following way
C
C Skip the include 'flib.fi' and 'flib.fd'
C Replace the original subroutine chkkey by the following
C dummy routine:
C
C Subroutine chkkey(code)
C integer*2 code
C code=0
C return
C end
C
C End of programmers information
C
C FEBRUARY 1999
C Two new keywords, ZEROSET and KREDUCT, are introduced. See
C keyword list below. KREDUCT may be used in order to save
C only the best trial solutions.It is presupposed then, that
C input data is very accurate and a cell axis is expected to
C be very long (>20 A)
C
C In order to avoid run time errors, a large number of small
C changes have been made.
C
C The earlier program versions were somewhat dependent on
C the wave-length used. The parameters: D1, D2 and SSQTL are
C now automatically ( i.e. if SELECT=-1 ,the default value)
C adjusted for WAVE. As in earlier program versions one can
C forget about WAVE if CHOICE=4, i.e. if input data are
C d-values.
C If correct WAVE is given, also the correct diffraction
C angles are reported in the output lists.
C
C Monoclinic solutions are checked for possible rhombohedral
C symmetry. If several high symmetry solutions are found, it
C is recommended to decrease the parameter VOL in order to
C find the smallest monoclinic cell (1/6 of the 'true' hexa-
C gonal cell). Then treor will check if the true symmetry is
C likely to be rhombohedral and calculate the possible
C hexagonal axes.
C
C SEPTEMBER 1997
C (Below 1997 is changed to 1999 (changed february 1999)
C Keywords (see below) may be written in upper or lower case.
C
C The program will run in 1999 mode if the keyword
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C SELECT has the value -1 (default value)
C
C The normal TREOR99 run is:
C
C Title line: Any text in col. 2-80
C Data lines: Less than 99 lines (Normally 20-25 lines).
C Free format.
C Only one value on each line is necessary.
C Optionally an intensity may be given as a
C second data on the line. Intensity data is
C not used by the program and only transferred
C to the output as max. 4 digits integers
C
C A blank line:
C choice=4, (if D-values were used on the data lines)
C Do not forget the , before next key-word
C Key-words may be given in arbitrary order
C end* and on arbitrary lines but the end* must
C be the last one.
C
C Usually no other key-words than CHOICE need to be changed
C from the default values.
C
C If a solution is found the program will automatically
C decrease NIX or increase MERIT and rerun the problem in
C order to check if a better solution can be found. However,
C triclinic tests will only be made if the first solution
C was triclinic.
C
C If no solution is found the program will automatically
C change the parameters IDIV and the error limits D1 and D2
C i.e. add 0.0001*(Wave/1.5405981)**2)and rerun the problem.
C
C Of course the TREOR99 mode may take a minute more on a
C Pentium but it is a strongly recommended, simple, safe and
C powerful procedure.
C
C Powder indexing depends to 95 per cent on the data quality
C If you are using a Pentium processor the CPU time will
C probably never exceed 3 minutes. ( A PC 486 may be almost
C ten times slower.)
C
C It is possible to run the program in TREOR4, TREOR90 or
C TREOR99 mode
C
C TREOR4 mode if VOL=positive value and SELECT is zero (or
C more.)
C TREOR90 mode if VOL=negative value and SELECT is zero (or
C more)
C TREOR99 mode if SELECT=-1 (Default) (Normally preferred
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C mode)
C If the TREOR99 mode is used, you normally only need to
C choose the correct CHOICE parameter.
C
C In all modes most of the key-word parameters may be
C changed from the default values ( c.f. the key-word list
C below).
C Do not change default values without good reasons. For
C example do not change VOL from the default value, unless
C you have reason to believe that the unit cell volume is
C more than 2000 A**3 ( You will not reduce CPU time much if
C you are using a VOL that is less than 2000 A**3)
C
C If TREOR99 finds a plausible solution ( according to the
C NIX and MERIT parameters) this will be announced on the
C display and the user may ( although not recommended )
C interrupt the calculations and look at the condensed
C output list.
C Interrupt...Press the letter i on the keyboard.
C If the program is running on a Pentium there is no reason
C for doing so.
C (The interrupt function is at present only available in the
C PC version.)
C
C Problem notes:
C
C A solution that is very close to a higher symmetry may be
C lost in the condensed output list, although an acceptable
C lower symmetry solution may be reported in the long output
C list. This may happen if two cell dimensions are almost
C equal.
C
C
C JUNE 1995
C Within this section JUNE 1995 to JUNE 1992 a very short
C description for the lazy user of TREOR90 (who does not want
C to read the complete documentation file) is given.
C
C The normal TREOR90 run is:
C
C Title line
C Data lines (20-25 lines, only one d-value, col.1-16, on each
C line)
C A blank line
C CHOICE=4, (if D-values were used on the data lines)
C SELECT=0, (to avoid the TREOR99 mode)
C VOL=-2000, (note the minus sign. --- a treor90 run)
C END* (stop card)
C
C It is now possible to interrupt the calculations. This can
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C be done by the letter i on the keyboard. Then the program
C will stop soon. The reason for this option is that one
C should never hesitate to give VOL eq. a negative value i.e.
C the most efficient test of all symmetries. One can always
C stop for example triclinic tests from the keyboard. (This
C option is only available on the PC version of the program)
C
C If no solution is found rerun the problem, but include the
C following keyword line:
C D1=0.0003, D2=0.0005,
C (note the , after each keyword value)
C Another test is to set
C IDIV=0,
C which means that the first seven lines will not be changed
C by ( what treor may erronously judge as ) higher order lines
C The parameters MERIT and NIX may also be changed. ( See
C below.) The first accepted solution may not be the best one.
C Therefore, follow the instructions on the condensed output
C file.
C Do not print the long output file. Use your editor and look
C for the most promising M-TEST lines.
C
C This program should be used to find a physical plausible
C solution of the indexing problem. The refinement is only
C preliminar ( not Hess weighted). Especially lines at high
C diffraction angles may be unindexed by treor.
C In final refinements all lines, all extinction conditions,
C Hess weights ( i.e. all diffraction angles should be given
C equal weights)and all knowledge about intensity distribution
C between overlaps ( if available) should be used.
C From this department a flexible dialouge program,(version
C 930101 of PIRUM) may be distributed.
C Program NBS*AIDS83 is (probably ?) recommended by ICDD.
C
C JUNE 1992
C It is strongly recommended to run TREOR90 on a PC/AT using a
C 486 CPU. Otherwise the VAX version TREOR90V may be used.
C AUGUST 1990
C OBS. In the PC/AT and VAX versions the subroutines ORTAL, MAEG
C and COUNT are not vectorized. Vectorized versions of these
C subroutines are available for CONVEX computers.
C The original TREOR90 has been written for a CONVEX vector
C processor. This should be kept in mind when the comments
C below are read. The program may be very time-consuming on a
C PC (unless a 486 processor is used).
C
C 1) Dominant zone test is added for the orthorhombic symmetry.
C 2) Dominant zone test is added for the triclinic symmetry.
C 3) Higher order lines among the first seven lines ( used in the
C base line sets) are automatically excluded from the trial
```

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C phase of the calculations.
C 4) If a monoclinic or triclinic solution is found, the program
C will end with a unit cell reduction followed by a conversion
C of the reduced cell to a conventional cell according to the
C metric symmetry. The reduction should be valid unless syste-
C matic extinctions are found in the trial cell.
C 5) If a satisfactory solution is found, only the condensed out-
C put file is needed. It contains all relevant information and
C only one indexed list.
C 6) The general output list (that is normally not needed, cf. 5)
C will only list trials where M20 ( or Mxx if less lines are
C available) is 6 or more and not more than 3 lines among the
C first 20 (or xx) lines are unindexed.
C 7) If the parameter VOL is given with a negative sign all symme-
C tries are tested until a final solution is found- if possible.
C OBS. This is the normal procedure for TREOR90
C 8) An algoritm for successive reduction of trial-cell volumes is
C used in monoclinic and triclinic tests if a negative VOL
C parameter is given. It is based on the input cell volume
C limit and the number of trial cells found with IQ ( See
C keyword IQ) or more than IQ indexable lines.
C 9) It is strongly recommended to give only the first ( well
C checked and accurately measured ) 25 lines in the diffraction
C data list (See LINE SET TWO).
C 10) It is expected that more than 95 per cent of monoclinic and
C higher symmetry patterns and probably more than 50 per cent
C of triclinic patterns will be indexed PRESUPPOSED the DATA
C QUALITY is high ( i.e. average differences between calculated
C and observed diffraction angles less than 0.02 deg. and also
C the weak lines included in the data). The experience of tri-
C clinic patterns is limited, however.
C 11) Obs. It is important to check cubic, tetragonal and hexagonal
C solutions by a second run with KS=0 and THS=0 ( See key-word
C list.) Do not trust cubic, tetragonal or hexagonal solutions
C without an orthorhombic test.
C 12) The reason for testing the symmetries in correct order ( from
C cubic to triclinic) and to START the orthrhombic, monoclinic
C and triclinic tests with dominant zone tests is that by this
C procedure false solutions are avoided.
C 13) For a normal TREOR90 run only the keywords
C
C CHOICE=X, (see key-word list)
C VOL=-2000, (OBS. The negative sign.)
C END*
C
C should be given after the diffraction data list. Computing
C times of more than 1 minute is rare for monoclinic or higher
C symmetries on a CONVEX computer. Computing times of more than
C 5 minutes (on a CONVEX) for a triclinic pattern has not yet
C been found. For a VAX (Micro VAX II) computing times may be
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C more than 50 times longer. The PC/AT 486 is faster than the
C Micro Vax II (but slower than CONVEX. The source code for VAX
C is not exactly the same as for CONVEX. There are very small
C differences between the PC/AT and the VAX versions, however.
C The input of file names and OPEN statements must be changed
C if you want to run this program on a VAX. Furthermore, the
C VAX version uses a subroutine to measure the CPU-time.
C 14) The input format for LINE SET TWO ( See below) is changed in
C agreement with the output format of the diffraction data file
C from the Guinier-H{gg film scanner system ( at Stockholm
C University). The change is mainly of interest for output of
C intensities.
C 15) The original key-word instructions given below are relevant
C as long as a positive VOL parameter is given.
C 16) If VOL is given a negative value (see 13 above) the following
C key-words are fixed: MONO=135 and MONOSET=7. Other key-words
C may be used as in the description below.
C 17) On the output lists
C M-TEST= xx UNINDEXED IN THE TEST= y
C usually means that xx is identical with M(20) and y is the
C number of unindexed lines whithin the first 20 lines ( i.e.
C used for the MERIT test). If less than 20 lines are available
C xx and y refer to the number of lines used.
C
C
C November 1988
C
C 29 11 88
C
C Trial-and-error program for indexing of unknown powder patterns.
C
C Cubic, Tetragonal, Hexagonal, Orthorhombic, Monoclinic and
C Triclinic symmetries.
C
C Version 2 1/9-75 = Version 26/4 plus
C
C DENS,EDENS and MOLW. See Keyword list below.
C
C Version 3 8/5-80 New output form
C
C Version 4 2/10-84 = Version 3 plus
C
C The following new options....
C
C 1. IDIV. See keyword IDIV below.
C 2. Monoclinic (020)-test
C Ref: Smith,G.S. and Kahara,E J.Appl.Cryst.
C 8 (1975) 681
C 3. SHORT. See keyword SHORT below.
C Short axis test. (Indexing of dominant zones.)
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C 4. TRIC. See keyword TRIC below.
C Indexing of triclinic patterns.
C
C The source code was modified in order to decrease the CPU-times
C in September 1988. The changes have no influence on input or out-
C put from the program, but CPU-time reductions of 20-50 per cent
C have been observed.
C
C Version 5. (=Version November 1988) 29/11 1988
C
C Dominant zone test introduced also for orthorhombic symmetry.
C In version 4 high symmetry short axis solutions were only found
C indirectly from the monoclinic tests.
C Condensed output file.
C A complete list of observed and calculated lines is only given
C for the solution (if it is found) i.e. for an indexing where the
C stop limits ( See keywords MERIT and NIX ) are fullfilled.
C Normally only the condensed output file is needed.
C If the stop limits are fullfilled the unit cell is refined three
C cycles more. OBS. Final least-squares refinement should be made
C by a separate program (for example by PIRUM). The TREOR program
C is written in order to FIND a plausible cell, not to produce the
C ultimate refinement.
C Only the first part of the difference analysis table is printed
C if no solution is found. (Usually it is not needed as you should
C rerun the problem after modifications of the input data.)
C
C If you have any questions, write to....
C
C P.-E.Werner
C Dept. of Structural Chemistry
C Arrhenius Laboratory
C Stockholm University
C S-106 91 Stockholm,
C SWEDEN
C
C
C
C TEL: 08 / 16 23 93
C FAX: 46-8-15 21 87
C Bitnet: WERNER@STRUC.SU.SE
C
C
C It is believed, however, that the following documentation should
C be sufficient for all careful readers.
C
C GOOD LUCK!
C
C
C
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C R E F E R E N C E S
C
C
C Basic principles. Werner,P.-E., Z.Kristallogr. 120 (1964) 375-387
C
C TREOR, a semi-exhaustive trial-and-error powder indexing program
C for all symmetries. Werner,P.-E., Eriksson,L. and Westdahl,M.,
C J. Appl. Crystallogr. 18 (1985) 367-370
C
C Refinement of unit cell. Werner,P.-E.,Arkiv Kemi 31(1969) 513-516
C
C Figure of merit. De Wolff,P.M.,J.Appl.Crystallogr. 1(1968)108-113
C
C Geometrical ambiguities. Mighell, A.D. and Santoro, A., J. Appl.
C Crystallogr. 8 (1975) 372
C
C
C G E N E R A L C O M M E N T S
C
C This is a general trial-and-error indexing program for X-ray
C diffraction powder patterns (i.e. all symmetries included).
C
C Historical information ---- In order to reduce computing times on
C computers without hardware floating point processers, parts of
C the program have been written for integer calculations.
C
C The parameters given as normal values in the keyword list below
C should be regarded as an important part of the program. They are
C based on experience from many successful runs on structures con-
C firmed by single crystal data.
C The parameters VOL and CEM, however, may be selected for the
C actual data set and the symmetry tried.
C ...For a monoclinic trial the parameter MONO must be non-zero.
C ...For a triclinic trial the parameter TRIC must be 1.
C A TREOR99 run (i.e. SELECT=-1) or a TREOR90 run (i.e. VOL= a nega-
C tive number) will automatically check all symmetries.
C
C Most of the powder patterns used to check the program have been
C obtained by focusing Guinier-Hagg cameras. The photographs have
C been measured by....
C 1. The method described by Hagg,G., Rev.Sci.Instr.18 (1947) 371
C and Westman,S. and Magneli,A., Acta Chem. Scand. 11 (1957) 1587
C 2. The method described by Malmros, G. and Werner, P.-E., Acta
C Chem. Scand. 27 (1973) 493
C 3. The film scanner system SCANPI ( written for the Guinier
C film scanners LS18 and LS20)
C The program has also been tested on a large number of NBS-data
C sets. (JCPDS data sets.)
C
C The accurate data obtained by NBS,National Bureau of Standards,
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C is clearly sufficient for successful indexing (in spite of the
C fact that they are now usually obtained by powder diffracto-
C meters. Unfortunately, however, many diffractometer data sets
C found in the litterature show parabolic deviations between
C observed and calculated diffraction angles.)
C
C The following citations, however, should be emphasized....
C
C 'The paramount importance of resolution for indexing work
C explains the high success rate for focussing camera data,
C especially from Guinier-Hagg instruments, whose resolution can
C omly be described as superb. It is rather less common ( and
C considerably more expensive) to obtain as good resolution with
C diffractometer data.'
C
C 'Powder indexing is not like structure analysis, which works
C well on good data, and will usually get by on poor data given
C a little more time and attention. Powder indexing works
C beautifully on good data, but with poor data it will usually
C not work at all'
C
C
C Ref: Data accuracy for powder indexing.Shirley,R.NBS Spec. Publ.
C 567 (1980) P.370 and P.362 respectively.
C
C WARNING!
C A zero point error is much more serious than statistical errors
C of the same magnitude.
C
C Sigma(Two theta) should be less than 0.02 deg.
C
C
C
C ******************************************
C * DO NOT WASTE COMPUTER TIME ON BAD DATA. *
C ******************************************
C
C An indexing algorithm cannot be statet rigorously because of
C the unpredictable distribution of unobserved lines and the
C errors of measurements. One (or two) impurity lines may cause
C severe problems.More impurity lines may rule out the possibility
C to index the pattern. Therefore, it is expected that various
C methods may be useful for various powder patterns. For example,
C a multitude of non-systematic extinctions may not appreciably
C affect the power of trial-and-error methods.
C
C The least-squares refinement of the unit cell dimensions should
C normally not be considered as the ultimate refinement. The main
C purpose of this program is to FIND the unit cell. The program
C PIRUM (version 930101) may be used for ultimate refinements.
```

```
C PIRUM (version 930101) is a dialouge version of the old PIRUM
C ( cf. ref. /Refinement of unit cell/ given above. ) Extinction
C conditions, Hess weights and max. accepted deviations between
C observed and calculated 2theta in degrees are normally used in
C version 930101 of PIRUM. In old PIRUM versions, parameters like
C D1, D2, and SSQTL (See keyword list below) were used.
C (cf. also the NBS*AIDS83 program. PIRUM is designed to be more
C user-friendly, however.)
C
C A limited number of nonsense cells may be printed on the output
C file. You should look for max. De Wolff figure of merit ( not F-
C index) and min. number of unindexed lines.
C
C WARNING. You should not accept unindexed lines unless you are
C able to explain them. On the other hand, you should not put in
C uncertain (doubtful) lines in this program. They may be tested
C later by a refinement program (ex. PIRUM).
C
C
C
C
C I N P U T D A T A
C
C
C LINE ONE. TITLE Any text in col.2-80
C
C
C LINE SET TWO. One SQ and optionally INTENSITY on each line.
C (Free format)
C SQ (=Sine square theta). It is also possible
C to use other types of input data. See keyword
C CHOICE
C
C The SQ data must be given in order, starting
C with the low order lines.Generally the first
C 20-25 lines should be used. Remainging lines
C (if any) may be used in later final refine-
C ments. (Program PIRUM).
C
C INTENSITY data is optional. It is never used
C by the program. If present, it will only be
C transferred to the output lists as (max.) 4
C digits integers.
C
C
C STOP LINE FOR LINE SET TWO IS A BLANK LINE (OR A NEGATIVE SQ)
C
C
C LINE SET THREE. GENERAL INSTRUCTIONS.
C
```

```
C All parameters in line set three have preset values.
C A preset value is denoted 'NORMAL VALUE 'below.
C Any 'NORMAL VALUE' may be changed in the following way:
C
C KEYWORD1=VALUE1, KEYWORD2 = VALUE2,
C KEYWORD3=VALUE3, ……., END*
C
C 1. The keywords are listed below
C 2. You must not forget =
C 3. The value may be given in free format ( integer or real ).
C 4. You must not forget ,
C
C You may use arbitrary positions on the lines.
C All blanks are irrelevant.
C The number of lines is arbitrary. You may give one or more
C key-word(s) on each line.
C
C Line set three must end with the keyword END* (OBS. asterisk)
C
C
C
C S T R A T E G Y
C Unless SELECT=-1 (i.e. TREOR99 mode) or VOL=(a negative value)
C (i.e. TREOR90 mode), the program will not differ much from
C earlier program versions. See the comments on the top of this
C list. Then (if VOL=negative value) only parameters such as NIX,
C MERIT, IDIV and in exeptional cases D1, SSQTL and/or D2 may be
C changed if indexing is not successful. Usually the main problem,
C however, is the quality of your diffraction data.
C Therefore, if the first run does not give a satisfactory
C solution, it may be recommended to increse D1 and D2 to 0.0003
C and 0.0005, respectively.
C
C If the TREOR99 mode is used (i.e. SELECT=-1) the program will,
C regardless a plausible solution is found or not, rerun the
C problem and automatically adjust some parameters. Therefore it
C is generally not necessary for the user to change the default
C values in MERIT, NIX, D1 and/or D2.
C
C If you are not using the normal TREOR99 procedure (i.e. SELECT=
C -1) or the TREOR90 procedure(i.e. negative VOL) the standard
C procedure is to start with the higher symmetries:
C cubic, tetragonal, hexagonal and orthorhombic ( in one run).
C Next the monoclinic symmetry may be tried. More than one job
C may be needed..successively increasing the number of base line
C sets, and cell volume (See keywords: VOL, CEM and MONOSET)
C
C If formula weight and density are known, they may be used. (See
C keywords: DENS, EDENS and MOLW). The CPU-time needed will then
C usually be strongly reduced. (Unfortunately they are usually
```

```
C not known and therefore they have not been used very much.)
C
C
C
C LINE SET THREE EXAMPLES: (TREOR4, not normal TREOR99 or TREOR90
C examples.)
C
C EXAMPLE 1.Next line (except C in col.1) represents a line set 3
C END*
C
C Cubic, tetragonal, hexagonal and orthorhombic symmetries are
C tried. It may be recommended to try a smaller VOL limit even if
C a solution with acceptable figure of merit has been obtained.
C Sometimes it is difficult to find the necessary transformations
C between a high symmetry unit cell of too large dimensions and
C the primitive one.
C
C
C EXAMPLE 2. Next two line is a line set 3.
C KS=0,THS=0,OS1=0,
C CEM=20, V O L = 1000 , MONO=130,END*
C
C This is an example of a first monoclinic trial. ( See keyword
C MONO). Note that it is irrelevant if you give 'CEM=20.0' or
C 'CEM=20' etc.
C
C
C EXAMPLE 3. Next.....etc.
C KS=0,THS=0,OS1=0,
C CEM=20, VOL=1500, MONO=130, END*
C
C If example 2 is unsuccessful you may increase the VOL parameter
C to 500
C
C
C EXAMPLE 4. Next.....etc.
C KS=0,THS=0,OS1=0,CEM=20,
C MONOSET=7,LIST=1,
C DENS=3.123,EDENS=0.2,MOLW=234,
C END*
C
C If you have any possibility to put in density and formula
C weight, the CPU-time will be much reduced. This may also be
C tried if you expect that the lattice contains a dominant zone
C i.e. if in a test run you get a large number of trial cells
C when using the keyword SHORT=1.
C
C
C
C EXAMPLE 5. Next....etc.
```

```
C CEM=20,VOL=700,TRIC=1,MERIT=20,END*
C
C This is a triclinic test ( OBS. time-consuming) ( See. keyword
C TRIC). A de Wolff figure merit of 20 may (sometimes) be needed
C for a triclinic cell
C
C The examples given above illustrate a step-wise strategy for
C indexing. However, the VOL parameter may be estimated from the
C D-value of the 20th line. (cf. keyword TRIC)
C
C
C WARNING. If the unit cell has a small volume, for example
C 250 A**3 and VOL=2000 is used, the correct solution
C may be lost in the trial process. The reason is that a
C large number of large trial cells may erroneously
C index more lines than the correct cell.
C The problem is less severe in TREOR90 as a negative
C VOL parameter will cause the program to test ( for all
C but the triclinic symmetry) half the maximum volume in
C a first step.
C
C WARNING. Estimation of the unit cell volume from the relations
C VOL(monoclinic cell)= 20*D(20)**3 where D(20)= the D-
C value for line number 20, and VOL(orthorhombic) =
C 31*D(20)**3 are much less reliable than the correspon-
C ding relation for the triclinic symmetry.
C VOL(triclinic)=13.39*D(20)**3
C Triclinic structures have no systematic extinctions!
C For structures containing atoms with large differences
C in scattering factors ( eg. metal-organic structures)
C the general rule may fail also in a triclinic case.
C Ref: Smith,G.S. J Appl. Crystallogr. 10 (1977) 252
C
C
C It is usually easy to put in a known ( or expected ) cell edge
C into the program. Example: A monoclinic trial with the restric-
C tion that one cell axis is X.XX A. Add this D-value in line set
C two. Suppose it will be line number 2. Then set MH2=1, MK2=1,
C ML2=0 and MS2=1. Then the line will be used as A-axis or ( the
C unique) B-axis in the monoclinic test.
C Conclusion: It is usually easy to put in prior knowledge and
C constraints -for example density- into the program. ( This
C statement is made because of some misunderstandings in the
C literature.)
C
C
C
C
C H O W T O I N T E R P R E T T H E O U T P U T.
C
```

```
C As in all good detective stories, the solution of the problem
C will usually be given on the last page.....
C i.e. the output list will be interrupted as soon as a unit
C cell that will satisfy the criteria set by the keywords NIX
C and MERIT are fullfilled. The main rule is that if all the
C first 20 lines are indexed and the De Wolff figure of merit
C M(20) is greater than 9, then the indexing problem is in
C principle solved. This does not mean that the cell is reduced,
C that a cell axis may not be double etc.,
C
C
C
C UNIT CELLS OBTAINED BY THE PROGRAM SHOULD BE CAREFULLY CHECKED
C
C A. If M(20) is less than 10 or more than one line is unindexed
C within the 20 first observed lines the solution is probably
C meaningless. Is any low-order line wrong ?
C B. Check for common factors in the quadratic forms.
C Example: A teragonal pattern may have H*H + K*K = 5*N
C i.e. the A-axis is 2.3607 ( square root of 5) times shorter
C than given on the output list.
C Example: If all H, K or L are even, the corresponding cell
C axis should be divided by 2.
C C. If the unit cell obtained is centered, derive a primitive
C cell. ( Run program MODCELL or a corresponding NBS program)
C D. Reduce the primitive cell and derive the conventional cell.
C (Run program REDUCT or a corresponding NBS program)
C E. Hexagonal and tetragonal cells are sometimes indexed as
C orthorhombic. Example: A=B*1.7321 i.e. a possible hexagonal
C cell.
C F. Check for geometrical ambiguities. See reference above. It
C is also strongly recommended to chech cubic, tetragonal and
C hexagonal solutions by an orthorhombic test. Put KS=0 and
C THS=0 and re-run the problem.
C There are two reasons for this procedure....
C 1. It may help you to identify geometrical ambiguities.
C 2. It has been found that sometimes very small orthorhombic
C unit cells can be indexed in an acceptable way ( i.e.
C fullfill the De Wolff criteria) by a larger unit cell of
C higher symmetry. Although the unit cells are sometimes
C related to each other, the relations are often difficult
C to detect, and therefore it is often convenient to let
C the program derive both solutions.
C G. The De Wolff figure of merits are derived from the assump-
C tion that no systematic extinctions are present and that
C all lines are indexed. A high figure of merit has no meaning
C unless all lines are indexed. The De Wolff figure of merit
C will increase in the final refinement made with program
C PIRUM, where the systematic extinctions can be taken into
C account.
```

```
C H. If possible, use the density and formula weight to check
C that the unit cell contains an integral number of formula
C units.
C I. If a cell axis is more than 20 A....be suspicious!
C It has been found that the De Wolff figure of merit may
C fail in such cases. (Require M(20) > 20)
C J. If one cell edge is much shorter than the others.....be
C suspicious! It may be a dominant zone problem and the De
C Wolff test may fail. (This problem is usually not severe in
C TREOR90, where short axis tests are made prior to the
C general tests.)
C K. If a table starts with...NOT REFINED UNIT CELL...
C two parameters are probably almost identical ( the symmetry
C may be higher) and the trial cell parameters are used to
C print the list.
C L. If no satisfactory solution is found ( See the keywords NIX
C and MERIT), the program may end with a small table con-
C taining a difference analysis. The program is described in
C Z. Kristallogr.120 (1964) p.381-382 (Werner,P.-E.) where it
C is named I1. The most interesting differences are those
C that have high multiplicities (on the top of the list) and
C are not too small (to the right of the list). In the present
C state of the program, the difference table is usually not
C needed.
C M. Why not solve the crystal structure from your powder data ?
C This is the ultimate way to prove the unit cell!
C
C
C
C
C
C
C
C K E Y W O R D L I S T
C
C KEYWORD. NORMAL COMMENT.
C VALUE.
C
C
C KH =4 Max H for cubic base line.
C KK =4 Max K for cubic base line.
C KL =4 Max L for cubic base line.
C
C OBS. The program will only generate
C H greater than or equal to K and
C K greater than or equal to L for
C this line.
C
C KS =6 Max H+K+L for this line.
C
```

```
C OBS. If KS=0 cubic test omitted.
C
C OBS. The cubic base lines are (1) and (2).
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C THH =4 Max H for tetragonal and hexagonal base lines.
C THK =4 Max K for tetragonal and hexagonal base lines.
C THL =4 Max L for tetragonal and hexagonal base lines.
C
C OBS. The program will only generate
C H greater than or equal to K for these lines.
C
C THS =4 Max H+K+L for these lines.
C
C OBS. If THS=0 tetragonal and hexagonal tests
C omitted.
C
C OBS. The tetragonal and hexagonal base lines
C are (1,2),(1,3) and (2,3)
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C OH1 =2 Max H for the first orthorhombic base line.
C OK1 =2 Max K for the first orthorhombic base line.
C OL1 =2 Max L for the first orthorhombic base line.
C
C OBS. The program will only generate
C H greater than or equal to K, and
C K greater than or equal to L for this line.
C This is also valid if the SELECT parameter
C is used. (See below).
C
C OS1 =3 Max H+K+L for this line.
C
C OBS. If OS1=0 orthorhombic test omitted.
C
C OH2 =2 Max H for the second orthorhombic base line.
C OK2 =2 Max K for the second orthorhombic base line.
C OL2 =2 Max L for the second orthorhombic base line.
C OS2 =4 Max H+K+L for this line.
C
C OH3 =2 Max H for the third orthorhombic base line.
C OK3 =2 Max K for the third orthorhombic base line.
C OL3 =2 Max L for the third orthorhombic base line.
C OS3 =4 Max H+K+L for this line.
C
C OBS. The orthorhombic base lines are
C (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) and (1,2,6)
C if SELECT0=0 (See SELECT below)
```

```
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C MH1 =2 Max Abs(H) for the first monoclinic base line.
C MK1 =2 Max K for the first monoclinic base line.
C ML1 =2 Max L for the first monoclinic base line.
C
C OBS. The program will only generate
C H greater than or equal to L for this line.
C EQ. TO L FOR THIS LINE.
C This is also valid if SELECT is used.
C (See SELECT below)
C
C MS1 =2 Max Abs(H)+K+L for this line
C The normal (and fast) way to test an expected cell
C axis is to put it in as SQ number one (in card set
C two) and set MH1=1, MK1=1, ML1=0 and MS1=1
C
C MH2 =2 Max Abs(H) for the second monoclinic base line.
C MK2 =2 Max K for the second monoclinic base line.
C ML2 =2 Max L for the second monoclinic base line.
C MS2 =3 Max Abs(H)+K+L for this line.
C
C MH3 =2 Max Abs(H) for the third monoclinic base line.
C MK3 =2 Max K for the third monoclinic base line.
C ML3 =2 Max L for the third monoclinic base line.
C MS3 =3 Max Abs(H)+K+L for this line.
C
C MH4 =2 Max Abs(H) for the fourth monoclinic base line.
C MK4 =2 Max K for the fourth monoclinic base line.
C ML4 =2 Max L for the fourth monoclinic base line.
C MS4 =4 Max Abs(H)+K+L for this line.
C
C OBS. The monoclinic base lines are
C (1,2,3,4) (1,2,3,5) and (1,2,4,5)
C If SELECT is less than 6. (See SELECT below)
C
C
C MONOSET =0 This parameter makes it possible to use more than 3
C base line sets in the monoclinic trials.
C If MONOSET is:
C Greater than 3, base line set (1,3,4,5) will be used
C Greater than 4, base line set (1,2,3,6) will be used
C Greater than 5, base line set (2,3,4,5) will be used
C Greater than 6, base line set (1,2,3,7) will be used
C Thus max 7 base line sets can be used.
C In N-TREOR (=STREOR), TREOR99 and TREOR90 modes
C MONOSET is fixed = 7
C
C MONOGAM=1 The best 5 trial parameter sets stored (See IQ)
```

```
C for each base line set will be refined before next
C base line set is tested.
C
C If MONOGAM=0 all base line sets are tried before
C any refinement is made.
C
C MONOGAM is only used in monoclinic tests.
C
C It is recommended to use MONOGAM=1 because a refined
C cell parameter set is always tested for the stop
C limits NIX and MERIT. Thus CPU-time may be saved.
C
C MONO =0 Max beta angle allowed in a cell.
C OBS. No monoclinic test if MONO=0
C (See also SHORT)
C In N-TREOR (=STREOR), TREOR99 and TREOR90 modes
C MONO is fixed = 135
C
C SHORT =1 Short axis test.
C The parameter is only used for monoclinic tests.
C The first six lines are tested for the occurrence
C of a common zero index in the six first lines.
C If SHORT=0 no short axis test.
C If you want to make this test without repeating
C other monoclinic tests, you may give MONO a
C negative sign.
C
C
C
C * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C
C USE =19 -or equal to the number of input lines if there are
C less than 19 lines,
C -or equal to the number of lines with sine square
C thetas less than 0.327
C -USE is the number of lines used in the trial-indexing
C part of the calculations.
C
C OBS. Max USE=20
C
C OBS. If you want to change USE, you should also
C change IQ. (See IQ).
C
C IQ =USE-3 The number of indexable lines required in the trial-
C indexing procedure if the cell should be stored for
C ev. least-squares refinement.
C These reciprocal cell parameters are printed if
C LIST=1
C
C LIST =0 See IQ above.
```

```
C
C SELECT =-1 In N-TREOR (=STREOR) and TREOR99 SELECT must be -1
C
C If you want to avoid the TREOR99 mode (but why ?..)
C set SELECT=0 or...
C
C if SELECT is positive the orthorhombic base lines
C are (SELECT,1,2) (SELECT,1,3) and (SELECT,2,3) or..
C
C if SELECT is greater than 5 the monoclinic base lines
C are (SELECT,1,2,3) (SELECT,1,2,4) and (SELECT,1,3,4)
C
C (Positive SELECT can not be used in TREOR99 mode.)
C
C
C MERIT =10 The De Wolff figure of merit required as stop limit.
C Ref: De Wolff,P.M. J. Appl. Crystallogr.
C 1 (1968) 108-113
C ( For cubic, tetragonal and hexagonal symmetries
C are the different quadratic forms as given in
C Int. Tabl. of X-Ray Crystallogr. (1968) Vol.2
C p.109-145 used in the calculation of the number of
C theoretical lines.)
C
C OBS. The figure of merit calculations are not
C strictly valid unless all 20 first lines are indexed.
C
C
C NIX =1 If a cell after least squares refinemnet has a figure
C of merit equal to or greater than MERIT and the
C number of not indexable lines among the USE first
C lines is less than or equal to NIX, the calculations
C are stopped.
C
C OBS. Otherwise he calculations will end with a
C difference analysis (Program I1. Werner,P.-E.
C Z.Kristallogr. 120 (1964) 375-378)
C (Now not very useful list. --'historical')
C
C IDIV =1 The 7 first lines are adjusted by (eventually
C occurring) higher order lines.
C If IDIV=0 no corrections.
C Usually the default value 1 is o.k. There are
C exeptions, however. If indexing is not
C successful, you may try IDIV=0
C
C WAVE =1.5405981 Wave length. (in Angstroem)
C As a rule one should not change WAVE
C If D-values are used in the input data file (See
C CHOICE=4) one can always pretend that WAVE was
```

```
C 1.5405981 A. WAVE is then a formal parameter only
C related to D1, SSQTL and D2 (See below).
C
C VOL =2000 Max cell volume (in Angstroem**3)
C A new option available in TREOR90 is to give a
C negative value of VOL, ex. VOL=-2000.
C See comments number 16 on the top of this list.
C
C CEM =25 Max cell edge (in Angstroem)
C The CPU-time is strongly dependent on VOL and CEM
C
C D1 =0.0002 (if WAVE=1.5405981) See D2 below.
C
C SSQTL =0.05 (if WAVE=1.5405981) See D2 below.
C
C D2 =0.0004 (if WAVE=1.5405981)
C A line is regarded as indexed if..
C sine square theta is less than SSQTL and
C Abs(sine square theta observed minus sine square
C theta calculated) is less than D1 or...
C if sine square theta is greater than SSQTL and
C the corresponding difference is less than D2.
C D1, SSQTL and D2 are used in the trial indexing
C part as well as in the least squares refinements
C If SELECT=-1 are D1, SSQTL and D2 automatically
C multiplied by the factor (WAVE/1.5405981)**2
C (i.e. D1, SSQTL and D2 depend on WAVE)
C
C
C CHOICE =0 Indicator defining SQ on card set two..
C CHOICE=0 SQ=Sine square theta
C =1 SQ=1/(D*D) (D-spaceing in Angstroem)
C =2 SQ=Theta (Theta=Bragg angle in deg.)
C =3 SQ=2*Theta
C =4 SQ=D
C OBS next line...
C CHOICE =4 Default value in N-TREOR (=STREOR)
C
C
C DENS =0 Density. (DENS=0 density not used.)
C If only an integral number of molecules in the unit
C cell is accepted DENS, EDENS and MOLW may be used.
C (On tour own responsibility)
C DENS = density in gram per cm**3
C
C EDENS =0 Not used unless DENS equals non zero.
C EDENS= Max deviation in DENS.
C OBS. DENS and EDENS are used in trial calculations
C i.e. they are used on non refined unit cells.
C Therefore, do not use too small EDENS
```

```
C
C MOLW =0 Not used unless DENS ( and EDENS ) are non zero.
C Mol. weight in A.U. (OBS. Crystal water included.)
C It is not recommended to use DENS, EDENS and MOLW
C in tests of orthorhombic and higher symmetries.
C
C
C TRIC =0 No triclinic test.
C If TRIC=1 all higher symmetry tests are omitted and
C a triclinic test is made.
C It is presupposed that all higher symmetries have
C been tried in earlier runs.
C Although it is in principle possible to index any
C pattern as triclinic, the indexing algorithm used
C here is not effective for higher symmetries.
C OBS. See comment 7 on the top of this list.
C TRIC is not used in N-TREOR (=STREOR), TREOR99 and
C TREOR90 modes.
C
C
C ZEROSET =0 This keyword may be given as an integer.
C ZEROSET*0.005 degrees are added to all theta-
C values (i.e. ZEROSET*0.01 deg. to all 2theta).
C Example: If 2theta-zero at 0.05 deg., then set
C ZEROSET=-5
C
C KREDUCT =0 If KREDUCT is given, only trial solutions with
C IQ=USE-(KREDUCT-1) number of lines indexed may
C be saved for trial-refinements.
C OBS. If KREDUCT=0 (or is not given) IQ=USE-3
C (See keyword IQ above)
C These reciprocal cell parameters are printed if
C LIST=1
C Thus, if KREDUCT=1 only trial-solutions where all
C lines are indexed will be saved for further tests.
C
C
C
C
C END* This keyword denotes the end of the parameter list.
C (i.e. end of card set three)
C
C
C
C
C C O M M E N T S F O R T H E P R O G R A M M E R
C
C
C THE FILES ARE OPENED IN THE MAIN PROGRAM (THE FIRST PROG).
C
```

```
C THE LOGICAL UNITS ARE..
C NUIT=9 THE CONDENSED OUTPUT FILE.
C IIN=8 THE DATA INPUT FILE.
C IOUT=7 THE OUTPUT FILE.
C NDISP=6 OUTPUT (ON DISPLAY) OF TRIAL PARAMETERS IF KEYWORD LIST=1
C (SEE KEYWORDS IQ AND LIST)
C LKEY=5 KEY-BOARD.
C THE LOGICAL UNIT NUMBERS 5,6,7,8 AND 9 ARE GIVEN IN THE MAIN
PROGRAM
C AND MAY BE CHANGED FOR YOUR COMPUTER. THEY NEED NOT BE CHANGED
IN
C ANY OTHER PLACE OF THE PROGRAM, HOWEVER.
C
C IF YOU ARE USING A VECTOR PROCESSOR THE VECTORIZED VERSION
C OF THE SUBROUTINES ORTAL, MAEG AND COUNT SHOULD BE USED.
C A SUBROUTINE NAMED HKLP SHOULD ALSO BE INCLUDED AND CALLED
C ONCE FROM SUBR. PWINL
C
C
C THE PROGRAM IS MAINLY WRITTEN IN FORTRAN (II) AND (IV), BUT
C FORTRAN 77 HAS BEEN USED TO SOME EXTENT. (SEE FOR EXAMPLE
SUBROUTINE
C TWODIM.)-IT IS THE INTENTION, HOWEVER, THAT IT SHOULD NOT BE
C DIFFICULT TO REWRITE THE FORTRAN 77 STATEMENTS IF ONLY FORTRAN(IV)
C IS AVAILABLE.
C
C VERSION 4 OF THE PROGRAM HAS BEEN DEVELOPED AT
C STOCKHOLM UNIVERSITY USING A VAX 11/750 COMPUTER.
C VERSION 5 WAS DEVELOPED FOR CONVEX 210, VAX 11/750 AND IBM PC/AT.
C VERSION TREOR90 IS WRITTEN FOR CONVEX 210. A NON-VECTORIZED
C VERSION IS ALSO AVAILABLE. TRICLINIC TESTS
C MAY BE VERY TIMECONSUMING ON A VAX, HOWEVER.
C
C CALLS FROM THE MAIN PROGRAM ARE TO...
C PWINL.....THE DATA INPUT ROUTINE.
C TREOB.....THE TRIAL MODULE (THE MOST TIME-CONSUMING PART).
C TREOC.....PROG. FOR DIFFERENCE ANALYSIS AND ORGANISATION FOR
TREOD.
C TREOD.....LEAST SQUARES REFINEMENTS OF THE BEST TRIAL CELLS.
C GET_CPU_TIME.....THIS SUBROUTINE MAY BE OMITTED. THEN THE CALLS
C FROM THE MAIN PROGRAM MUST BE SKIPPED. THE
C SUBROUTINE IS MACHINE DEPENDENT. NO OTHER
C PART OF THE PROGRAM IS MACHINE DEPENDENT.
C ON CONVEX THE DTIME ROUTINE IS USED.
C
C
C
C BELOW IS A LIST OF THE COMMAND FILE USED FOR
C THE VAX 11/750 AVAILABLE AT THE ARRHENIUS LABORATORY,
C UNIVERSITY OF STOCKHOLM, SWEDEN.
```

```
C
C
$INQUIRE/P TREDAT "TREOR INPUT DATA FILE"
$INQUIRE/P LIST "OUTPUT FILE"
$INQUIRE/P COND "CONDENSED OUTPUT FILE"
$INQUIRE/P TYPE "EXECUTE (E) OR BATCH (B)"
$IF TYPE .EQS. "B" THEN GOTO BATCH
$IF TYPE .EQS. "E" THEN GOTO START
$EXIT
$!
$START:
$ASSIGN 'LIST' LIST
$ASSIGN 'TREDAT' TREDAT
$ASSIGN 'COND' COND
$ON CONTROL_Y THEN CONTINUE
$ASSIGN/USER_MODE SYS$COMMAND: SYS$INPUT
$RUN TREOR
$DEASSIGN LIST
$DEASSIGN TREDAT
$DEASSIGN COND
$EXIT
$!
$BATCH:
$INQUIRE/P JOBNAME "JOB NAME"
$OPEN/WRITE JOB TREORJOB.TMP
$WRITE JOB "$SET NOVERIFY"
$WRITE JOB "$SET DEFAULT "F$DIRECTORY()'"
$WRITE JOB "$ASSIGN "LIST' LIST"
$WRITE JOB "$ASSIGN "TREDAT' TREDAT"
$WRITE JOB "$ASSIGN "COND' COND"
$WRITE JOB "$RUN TREOR
$WRITE JOB "$DELETE/LOG *.TMP;*
$WRITE JOB "$EXIT"
$CLOSE JOB
$SUBMIT/NOTIFY/NAME='JOBNAME'/QUEUE=SYS$BATCH TREORJOB.TMP
```

E N D O F P R O G R A M I N S T R U C T I O N S

T E S T E X A M P L E S (USING TREOR VERSION 4.)
NO CHANGES IN THE INPUT DATA ARE NEEDED FOR VERSION 5.

EXAMPLE 1. INPUT DATA..

```
NBS 25 SEC.17 P.77 SR2CR2O7
7.91
7.238
5.601
4.739
4.423
4.070
```

3.538
3.474
3.443
3.315
3.040
2.950
2.931
2.836
2.796
2.751
2.673
2.636
2.609
2.596
2.503
2.420
2.413
2.357
2.305

CHOICE=4,
END*

END OF INPUT DATA.
COMMENT. THE FIRST LINES GIVEN BY NBS ARE 7.91, 7.24, 5.601, 4.739,
4.070, 3.955, 3.619 ETC.
ACCORDING TO THE RULE GIVEN IN THE TREOR COMMENT LIST (SEE.
SECTION..INPUT DATA...LINE SET TWO)
THE LINES 3.955 (=7.91/2) AND 3.619 (=7.238/2) ARE OMITTED
IN THE TREOR RUN. THE LINE 7.24 IS ADJUSTED TO 7.238.

THE FOLLOWING IS THE OUTPUT LIST FROM TREOR....

TREOR (4)- 84 10 02
NBS 25 SEC.17 P.77 SR2CR2O7
7.910000
7.238000
5.601000
4.739000
4.423000
4.070000
3.538000
3.474000
3.443000
3.315000
3.040000
2.950000
2.931000
2.836000

2.796000
2.751000
2.673000
2.636000
2.609000
2.596000
2.503000
2.420000
2.413000
2.357000
2.305000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10 MAX NUMBER OF UNINDEXED LINES= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 25.0 MAX CELL VOLUME= 2000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
CUBIC TEST
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
TETRAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
K= 19 XY= 0.00474 0.00658

CYCLE RESULTS

0.004739 0.006598 0.000000 0.000000 0.000000 0.000000
0.004739 0.006598 0.000000 0.000000 0.000000 0.000000
0.004739 0.006598 0.000000 0.000000 0.000000 0.000000

NUMBER OF SINGLE INDEXED LINES= 21 TOTAL NUMBER OF LINES= 25
NUMBER OF SINGLE INDEXED LINES = 21
TOTAL NUMBER OF LINES = 25
A = 11.189680 0.001176 A ALFA = 90.000000 0.000000 DEG
B = 11.189680 0.001176 A BETA = 90.000000 0.000000 DEG
C = 9.482903 0.002338 A GAMMA = 90.000000 0.000000 DEG
UNIT CELL VOLUME = 1187.34 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
1 1 0 0.009488 0.009478 0.000010 11.180 11.174 7.9080
1 0 1 0.011323 0.011337 -0.000014 12.217 12.225 7.2390
2 0 0 0.018975 0.018956 0.000019 15.835 15.827 5.5920
0 0 2 0.026421 0.026393 0.000027 18.709 18.699 4.7390
2 1 1 0.030331 0.030293 0.000038 20.059 20.047 4.4230
1 1 2 0.035820 0.035871 -0.000051 21.820 21.835 4.0700
3 1 0 0.047403 0.047390 0.000013 25.150 25.147 3.5380

3 0 1 0.049165 0.049249 -0.000084 25.622 25.644 3.4740
2 1 2 0.050055 0.050088 -0.000034 25.856 25.865 3.4430
3 1 1 0.053995 0.053988 0.000007 26.873 26.871 3.3150
1 0 3 0.064205 0.064124 0.000081 29.356 29.337 3.0400
2 2 2 0.064305 29.379
3 2 1 0.068183 0.068205 -0.000022 30.273 30.278 2.9500
1 1 3 0.068863 30.427
3 0 2 0.069070 0.069044 0.000026 30.474 30.468 2.9310
3 1 2 0.073775 0.073783 -0.000009 31.521 31.523 2.8360
4 0 0 0.075900 0.075823 0.000077 31.984 31.967 2.7960
2 0 3 0.078404 0.078341 0.000063 32.521 32.508 2.7510
2 1 3 0.083046 0.083080 -0.000034 33.498 33.505 2.6730
3 3 0 0.085394 0.085301 0.000093 33.982 33.963 2.6360
4 1 1 0.087171 0.087161 0.000010 34.345 34.343 2.6090
3 2 2 0.088046 0.088000 0.000046 34.522 34.513 2.5960
4 2 0 0.094710 0.094779 -0.000069 35.847 35.861 2.5030
4 2 1 0.101318 0.101378 -0.000059 37.121 37.132 2.4200
3 0 3 0.101907 0.102036 -0.000129 37.233 37.257 2.4130
4 0 2 0.102217 37.291
3 1 3 0.106807 0.106775 0.000032 38.151 38.145 2.3570
4 1 2 0.106956 38.179
3 3 2 0.111680 0.111695 -0.000014 39.046 39.049 2.3050
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 29
M(20)= 32 AV.EPS.= 0.0000378
F 20 = 57.(0.009765, 36)
M(25)= 29 AV.EPS.= 0.0000424
F 25 = 54.(0.010122, 46)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(197<<9)60
0 LINES ARE UNINDEXED
CHECK IF THERE IS ANY COMMON FACTOR IN THE QUADRATIC FORMS
CHECK CONVERGENCE IN THE REFINEMENT (EV. USE PROGRAM PIRUM OR PURUM)
END OF CALCULATIONS
USED CPU-TIME= 3. SEC.

END OF THE OUTPUT LIST.
COMMENT. NOTE COMMENT F IN SECTION ..HOW TO INTERPRET THE OUTPUT..
THE ORTHORHMBIC CHECK (KS=0 AND THS=0) IS NOT INCLUDED HERE.
IF YOU RUN THE ORTHORHOMBIC TEST YOU WILL SEE THAT AN
IDENTICAL SOLUTION IS FOUND. (A NON REFINEABLE ORTHORHOMBIC
CELL WILL AUTOMATICALLY BE CONVERTED TO THE TETRAGONAL CELL)

EXAMPLE 2. INPUT DATA

NBS.25 SEC.17 P.7 NH4B5O8*4H2O
6.00

5.67
5.52
4.951
4.617
4.427
3.544
3.383
3.334
3.271
3.003
2.926
2.868
2.834
2.760
2.680
2.627
2.586
2.533
2.479
2.414
2.367
2.332
2.317
2.312

CHOICE=4,
END*

END OF INPUT DATA.
COMMENT. NOTE THAT IN ALL EXAMPLES THE 25 FIRST LINES (NOT MORE)
ARE INCLUDED IN THE INPUT DATA FILE.
THE FOLLOWING IS THE OUTPUT LIST FROM TREOR..
TREOR (4)- 84 10 02
NBS.25 SEC.17 P.7 NH4B5O8*4H2O
6.000000
5.670000
5.520000
4.951000
4.617000
4.427000
3.544000
3.383000
3.334000
3.271000
3.003000
2.926000
2.868000
2.834000
2.760000
2.680000

2.627000
2.586000
2.533000
2.479000
2.414000
2.367000
2.332000
2.317000
2.312000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10 MAX NUMBER OF UNINDEXED LINES= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 25.0 MAX CELL VOLUME= 2000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
CUBIC TEST
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
TETRAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
HEXAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
ORTHORHOMBIC TEST
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
K= 19 XYZ= 0.00462 0.00487 0.00696

CYCLE RESULTS

0.004620 0.004876 0.006953 0.000000 0.000000 0.000000
0.004621 0.004876 0.006955 0.000000 0.000000 0.000000
0.004620 0.004876 0.006956 0.000000 0.000000 0.000000

NUMBER OF SINGLE INDEXED LINES= 21 TOTAL NUMBER OF LINES= 25
NUMBER OF SINGLE INDEXED LINES = 21
TOTAL NUMBER OF LINES = 25
A = 11.333113 0.003438 A ALFA = 90.000000 0.000000 DEG
B = 11.031460 0.002297 A BETA = 90.000000 0.000000 DEG
C = 9.236147 0.003381 A GAMMA = 90.000000 0.000000 DEG
UNIT CELL VOLUME = 1154.71 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.

1 1 1 0.016449 0.016451 -0.000002 14.738 14.738 6.0060
2 0 0 0.018470 0.018479 -0.000009 15.622 15.626 5.6680
0 2 0 0.019473 0.019504 -0.000030 16.043 16.056 5.5200
1 2 0 0.024138 0.024123 0.000015 17.876 17.870 4.9580
0 0 2 0.027751 0.027823 -0.000071 19.179 19.204 4.6240
2 1 1 0.030276 0.030311 -0.000035 20.041 20.053 4.4270
0 2 2 0.047242 0.047326 -0.000084 25.107 25.130 3.5440
1 2 2 0.051846 0.051946 -0.000100 26.323 26.349 3.3830
3 1 1 0.053381 0.053409 -0.000028 26.717 26.724 3.3340
1 3 1 0.055457 0.055458 -0.000001 27.241 27.242 3.2710
2 2 2 0.065797 0.065805 -0.000008 29.726 29.728 3.0030
2 3 1 0.069306 0.069318 -0.000012 30.527 30.530 2.9260
3 0 2 0.069400 30.549
1 1 3 0.072137 0.072096 0.000041 31.160 31.151 2.8680
4 0 0 0.073879 0.073916 -0.000038 31.544 31.552 2.8340
3 1 2 0.074276 31.631
0 4 0 0.077893 0.078014 -0.000121 32.412 32.438 2.7600
1 4 0 0.082613 0.082634 -0.000021 33.408 33.412 2.6800
4 1 1 0.085748 34.055
2 1 3 0.085980 0.085956 0.000025 34.102 34.097 2.6270
3 2 2 0.088728 0.088904 -0.000176 34.660 34.695 2.5860
3 3 1 0.092480 0.092416 0.000064 35.409 35.396 2.5330
2 4 0 0.096553 0.096493 0.000060 36.206 36.195 2.4790
4 0 2 0.101823 0.101739 0.000084 37.217 37.201 2.4140
0 4 2 0.105906 0.105837 0.000070 37.984 37.971 2.3670
3 1 3 0.109109 0.109055 0.000055 38.576 38.566 2.3320
1 4 2 0.110527 0.110456 0.000070 38.836 38.823 2.3170
1 3 3 0.111005 0.111103 -0.000098 38.923 38.941 2.3120
0 0 4 0.111290 38.975
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 29
M(20)= 16 AV.EPS.= 0.0000469
F 20 = 27.(0.011589, 64)
M(25)= 14 AV.EPS.= 0.0000526
F 25 = 29.(0.012058, 74)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
CHECK IF THERE IS ANY COMMON FACTOR IN THE QUADRATIC FORMS
CHECK CONVERGENCE IN THE REFINEMENT (EV. USE PROGRAM PIRUM OR PURUM)
END OF CALCULATIONS
USED CPU-TIME= 41. SEC.

END OF THE OUTPUT LIST.
COMMENT. NOTE THAT THE LINES 6.00, 5.67, 4.951, AND 4.617 ARE ADJUSTED BY THE PROGRAM BECAUSE HIGHER ORDER LINES ARE AVAILABLE FOR ALL THESE LINES.
IF YOU WANT TO AVOID SUCH ADJUSTMENTS..GIVE IDIV=0..
IN THE INPUT LIST.

EXAMPLE 3. INPUT DATA

```
NBS.25 SEC.17 P.9 (NH4)2NI(SO4)2*6H2O
7.19
6.24
5.98
5.388
5.248
5.090
4.397
4.316
4.243
4.166
4.147
3.952
3.757
3.586
3.466
3.410
3.376
3.119
3.037
3.027
2.943
2.913
2.903
2.892
2.853

CHOICE=4,
VOL=1000, CEM=20,
KS=0,THS=0,OS1=0,
MONO=130,
END*

END OF INPUT DATA.
COMMENT. IT IS PRESUPPOSED THAT THE HIGH SYMMETRY TESTS
(I.E. CHOICE=4,END* ) HAVE FAILED.
THEN THIS IS THE NORMAL FIRST MONOCLINIC TEST.

THE FOLLOWING IS THE OUTPUT LIST FROM TREOR..

TREOR (4)- 84 10 02
NBS.25 SEC.17 P.9 (NH4)2NI(SO4)2*6H2O
7.190000
6.240000
5.980000
5.388000
5.248000
```

5.090000
4.397000
4.316000
4.243000
4.166000
4.147000
3.952000
3.757000
3.586000
3.466000
3.410000
3.376000
3.119000
3.037000
3.027000
2.943000
2.913000
2.903000
2.892000
2.853000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10 MAX NUMBER OF UNINDEXED LINES= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 20.0 MAX CELL VOLUME= 1000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
CUBIC TEST
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
TETRAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
HEXAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
ORTHORHOMBIC TEST
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
MONOCLINIC TEST
MAX BETA ALLOWED= 130 DEG.
(020)-SEARCH
K= 19 XYZU= 0.007666 0.003812 0.016593 0.006526

CYCLE RESULTS

0.007675 0.003815 0.016637 0.006583 0.000000 0.000000
0.007679 0.003814 0.016640 0.006579 0.000000 0.000000
0.007679 0.003814 0.016640 0.006579 0.000000 0.000000

NUMBER OF SINGLE INDEXED LINES= 20 TOTAL NUMBER OF LINES= 25
NUMBER OF SINGLE INDEXED LINES = 20
TOTAL NUMBER OF LINES = 25
A = 9.188087 0.001842 A ALFA = 90.000000 0.000000 DEG
B = 12.472351 0.004108 A BETA =106.917381 0.020982 DEG
C = 6.241651 0.001464 A GAMMA = 90.000000 0.000000 DEG
UNIT CELL VOLUME = 684.32 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
1 1 0 0.011478 0.011493 -0.000015 12.300 12.309 7.1900
0 2 0 0.015249 0.015257 -0.000009 14.187 14.191 6.2380
0 0 1 0.016593 0.016640 -0.000047 14.802 14.823 5.9800
0 1 1 0.020439 0.020454 -0.000015 16.439 16.445 5.3880
-1 1 1 0.021544 0.021554 -0.000010 16.881 16.885 5.2480
1 2 0 0.022903 0.022936 -0.000034 17.409 17.422 5.0900
2 0 0 0.030691 0.030715 -0.000025 20.179 20.187 4.3970
0 2 1 0.031853 0.031897 -0.000044 20.562 20.576 4.3160
-1 2 1 0.032959 0.032997 -0.000039 20.920 20.932 4.2430
-2 0 1 0.034189 0.034198 -0.000009 21.311 21.314 4.1660
0 3 0 0.034329 21.355
2 1 0 0.034503 0.034530 -0.000027 21.410 21.418 4.1470
-2 1 1 0.037991 0.038012 -0.000021 22.479 22.486 3.9520
1 3 0 0.042037 0.042008 0.000029 23.663 23.654 3.7570
2 2 0 0.045973 24.762
1 2 1 0.046142 0.046154 -0.000012 24.808 24.812 3.5860
-2 2 1 0.049393 0.049455 -0.000063 25.682 25.698 3.4660
0 3 1 0.051028 0.050969 0.000059 26.111 26.096 3.4100
-1 3 1 0.052061 0.052069 -0.000008 26.379 26.381 3.3760
0 4 0 0.060994 0.061030 -0.000036 28.597 28.605 3.1190
-1 0 2 0.061080 28.617
2 1 1 0.064332 0.064326 0.000006 29.386 29.384 3.0370
-1 1 2 0.064758 0.064895 -0.000137 29.485 29.517 3.0270
2 3 0 0.065044 29.552
-2 3 1 0.068508 0.068527 -0.000020 30.347 30.351 2.9430
1 4 0 0.068709 30.392
-3 1 1 0.069926 0.069828 0.000098 30.667 30.645 2.9130
0 1 2 0.070408 0.070373 0.000035 30.775 30.767 2.9030
-2 0 2 0.070945 0.070960 -0.000015 30.895 30.898 2.8920
3 1 0 0.072898 0.072924 -0.000026 31.328 31.334 2.8530
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 30
M(20)= 36 AV.EPS.= 0.0000322
F 20 = 73.(0.009822, 28)
M(25)= 28 AV.EPS.= 0.0000335
F 25 = 67.(0.009592, 39)

M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
CHECK IF THERE IS ANY COMMON FACTOR IN THE QUADRATIC FORMS
CHECK CONVERGENCE IN THE REFINEMENT (EV. USE PROGRAM PIRUM OR PURUM)
END OF CALCULATIONS
NUMBER OF CELLS WITH 16 OR MORE INDEXABLE LINES
IN MONOCLINIC (020)-TESTS 13 SOLUTIONS
IN MONOCLINIC DOMINANT ZONE TESTS 0 SOLUTIONS
IN MONOCLINIC GENERAL TESTS 0 SOLUTIONS
IN TRICLINIC TESTS 0 SOLUTIONS
USED CPU-TIME= 21. SEC.

END OF THE OUTPUT LIST.
COMMENT. NO GENERAL MONOCLINIC TESTS (OR SHORT AXIS TESTS) HAVE BEEN
MADE AS THE SOLUTION WAS FOUND BY THE DEDUCTIVE (020)-FINDING ALGORITHM.

EXAMPLE 4. INPUT DATA..

NBS.25 SEC.17 P.11 (NH4)2S2O3
5.480
5.093
4.741
4.553
4.386
4.257
3.501
3.469
3.353
3.248
3.199
3.046
3.010
2.925
2.915
2.785
2.739
2.629
2.612
2.582
2.569
2.547
2.536
2.500
2.453

CHOICE=4,
VOL=1000, CEM=20,
MONO=130,
KS=0,THS=0,OS1=0,
END*

END OF INPUT DATA.
COMMENT. CONDITIONS AS IN EXAMPLE 3 ABOVE.

THE FOLLOWING IS THE OUTPUT LIST FROM TREOR..

TREOR (4)- 84 10 02
NBS.25 SEC.17 P.11 (NH4)2S2O3
5.480000
5.093000
4.741000
4.553000
4.386000
4.257000
3.501000
3.469000
3.353000
3.248000
3.199000
3.046000
3.010000
2.925000
2.915000
2.785000
2.739000
2.629000
2.612000
2.582000
2.569000
2.547000
2.536000
2.500000
2.453000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10 MAX NUMBER OF UNINDEXED LINES= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 20.0 MAX CELL VOLUME= 1000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
CUBIC TEST
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
TETRAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)

BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
HEXAGONAL TEST
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 0
ORTHORHOMBIC TEST
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 0
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
MONOCLINIC TEST
MAX BETA ALLOWED= 130 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
K= 19 XYZU= 0.005717 0.014056 0.007738 0.001113

CYCLE RESULTS

0.005716 0.014053 0.007705 0.001085 0.000000 0.000000
0.005716 0.014056 0.007700 0.001080 0.000000 0.000000
0.005716 0.014056 0.007700 0.001080 0.000000 0.000000

NUMBER OF SINGLE INDEXED LINES= 21 TOTAL NUMBER OF LINES= 25
NUMBER OF SINGLE INDEXED LINES = 21
TOTAL NUMBER OF LINES = 25
A = 10.222344 0.001990 A ALFA = 90.000000 0.000000 DEG
B = 6.497315 0.001773 A BETA = 94.669502 0.020604 DEG
C = 8.807463 0.001939 A GAMMA = 90.000000 0.000000 DEG
UNIT CELL VOLUME = 583.03 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
1 1 0 0.019773 0.019772 0.000001 16.167 16.167 5.4780
2 0 0 0.022867 0.022865 0.000002 17.395 17.394 5.0940
-1 1 1 0.026398 0.026392 0.000007 18.701 18.699 4.7410
1 1 1 0.028624 0.028552 0.000071 19.481 19.456 4.5530
0 0 2 0.030845 0.030801 0.000044 20.230 20.216 4.3860
2 0 1 0.032742 0.032725 0.000017 20.850 20.845 4.2570
-1 1 2 0.048410 0.048412 -0.000003 25.421 25.421 3.5010
-2 0 2 0.049307 0.049345 -0.000038 25.659 25.669 3.4690
1 1 2 0.052778 0.052733 0.000045 26.563 26.551 3.3530
-3 0 1 0.055905 27.353
0 2 0 0.056245 0.056223 0.000023 27.438 27.432 3.2480
2 0 2 0.057982 0.057986 -0.000005 27.867 27.868 3.1990
0 2 1 0.063953 0.063923 0.000030 29.297 29.290 3.0460

3 1 0 0.065492 0.065501 -0.000010 29.655 29.658 3.0100
0 0 3 0.069353 0.069302 0.000051 30.538 30.526 2.9250
-3 1 1 0.069830 0.069961 -0.000131 30.645 30.675 2.9150
3 1 1 0.076501 0.076442 0.000059 32.113 32.101 2.7850
2 2 0 0.079092 0.079087 0.000005 32.668 32.667 2.7390
-2 0 3 0.085686 34.042
-1 1 3 0.085849 0.085834 0.000016 34.075 34.072 2.6290
0 2 2 0.086971 0.087024 -0.000053 34.304 34.315 2.6120
3 0 2 0.088728 34.660
2 2 1 0.089003 0.088948 0.000055 34.715 34.704 2.5820
-3 1 2 0.089906 0.089821 0.000085 34.896 34.879 2.5690
4 0 0 0.091466 0.091459 0.000007 35.208 35.206 2.5470
1 1 3 0.092261 0.092315 -0.000053 35.365 35.376 2.5360
-4 0 1 0.094838 35.872
1 2 2 0.094938 0.094900 0.000038 35.892 35.885 2.5000
2 0 3 0.098611 0.098648 -0.000037 36.604 36.611 2.4530
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 29
M(20)= 28 AV.EPS.= 0.0000332
F 20 = 51.(0.008314, 48)
M(25)= 26 AV.EPS.= 0.0000354
F 25 = 56.(0.008396, 54)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
CHECK IF THERE IS ANY COMMON FACTOR IN THE QUADRATIC FORMS
CHECK CONVERGENCE IN THE REFINEMENT (EV. USE PROGRAM PIRUM OR PURUM)
END OF CALCULATIONS
NUMBER OF CELLS WITH 16 OR MORE INDEXABLE LINES
IN MONOCLINIC (020)-TESTS 0 SOLUTIONS
IN MONOCLINIC SHORT AXIS TESTS 0 SOLUTIONS
IN MONOCLINIC GENERAL TESTS 13 SOLUTIONS
IN TRICLINIC TESTS 0 SOLUTIONS
USED CPU-TIME= 120. SEC.

END OF OUTPUT LIST.
COMMENT. NO SOLUTION WAS FOUND IN THE (020)- AND SHORT AXIS TESTS.
THE SOLUTION WAS FOUND BY THE GENERAL MONOCLINIC TESTS.

EXAMPLE 5. INPUT DATA.

NBS.25 SEC.17 P.64 K2S2O8
5.27
4.892
4.847
4.602
3.750
3.699

3.603
3.443
3.268
3.232
3.153
3.025
2.736
2.634
2.548
2.466
2.419
2.397
2.358
2.315
2.297
2.273
2.239
2.154
2.098

CHOICE=4,
CEM=20, VOL=500,
TRIC=1,
END*

END OF INPUT DATA.
COMMENT. IT IS PRESUPPOSED THAT HIGH SYMMETRY TESTS (CUBIC, TETRAGONAL,
HEXAGONAL AND ORTHORHOMBIC) AS WELL AS MONOCLINIC TESTS HAVE FAILED.
BY USING THE PARAMETER...TRIC=1...THE PROGRAM WILL GO DIRECTLY TO THE TRICLINIC TESTS.
D20=2.315 AND 13.39*(2.135**3)=130 IS THE ESTIMATED CELL VOLUME. (FOUND VOLUME=182 SEE. BELOW). IT IS REASONABLE TO ADD A FEW HUNDRED CUBIC ANGSTROEM FOR THE VOL PARAMETER.

THE FOLLOWING IS THE OUTPUT LIST FROM TREOR..

TREOR (4)- 84 10 02
NBS.25 SEC.17 P.64 K2S2O8
5.270000
4.892000
4.847000
4.602000
3.750000
3.699000
3.603000
3.443000

3.268000
3.232000
3.153000
3.025000
2.736000
2.634000
2.548000
2.466000
2.419000
2.397000
2.358000
2.315000
2.297000
2.273000
2.239000
2.154000
2.098000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10 MAX NUMBER OF UNINDEXED LINES= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 20.0 MAX CELL VOLUME= 500.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
TRICLINIC TEST
K= 19 A11-33= 0.024794 0.021381 0.014148 A12-23= 0.003980-0.010827-0.010179

CYCLE RESULTS

0.024733 0.021358 0.014199 -0.010851 0.004041 -0.010185
0.024732 0.021360 0.014204 -0.010857 0.004044 -0.010192
0.024732 0.021360 0.014204 -0.010857 0.004044 -0.010192

NUMBER OF SINGLE INDEXED LINES= 19 TOTAL NUMBER OF LINES= 25
NUMBER OF SINGLE INDEXED LINES = 19
TOTAL NUMBER OF LINES = 25
A = 5.117541 0.001495 A ALFA = 73.732178 0.028467 DEG
B = 5.511826 0.002494 A BETA = 73.916046 0.040242 DEG
C = 7.034377 0.002352 A GAMMA = 90.202797 0.030145 DEG
UNIT CELL VOLUME = 182.31 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
0 1 0 0.021381 0.021360 0.000021 16.816 16.808 5.2680
1 0 0 0.024794 0.024732 0.000062 18.119 18.096 4.8920
0 1 1 0.025351 0.025372 -0.000021 18.323 18.331 4.8380
1 0 1 0.028115 0.028079 0.000036 19.305 19.293 4.5940
-1 1 0 0.042195 0.042047 0.000147 23.707 23.665 3.7500
1 1 1 0.043366 0.043290 0.000076 24.039 24.018 3.6990
0 -1 1 0.045708 0.045755 -0.000048 24.690 24.703 3.6030

1 1 0 0.050055 0.050135 -0.000081 25.856 25.878 3.4430
1 -1 1 0.055559 0.055586 -0.000027 27.267 27.274 3.2680
0 0 2 0.056804 0.056816 -0.000012 27.577 27.580 3.2320
-1 1 1 0.056917 27.605
1 0 2 0.059686 0.059833 -0.000148 28.282 28.317 3.1530
1 1 2 0.064844 0.064854 -0.000010 29.505 29.507 3.0250
0 2 1 0.079266 0.079259 0.000007 32.705 32.703 2.7360
-1 -1 1 0.085388 33.981
0 2 0 0.085524 0.085438 0.000085 34.009 33.991 2.6340
2 0 1 0.091394 0.091416 -0.000022 35.193 35.198 2.5480
1 -1 2 0.097574 0.097533 0.000041 36.404 36.396 2.4660
1 2 1 0.101222 37.103
0 2 2 0.101402 0.101487 -0.000085 37.137 37.153 2.4190
-1 0 2 0.103272 0.103262 0.000010 37.490 37.488 2.3970
-1 2 1 0.106716 0.106760 -0.000043 38.134 38.142 2.3580
2 1 1 0.110718 0.110672 0.000045 38.871 38.862 2.3150
-2 1 0 0.112198 39.140
2 0 2 0.112314 39.161
1 2 2 0.112460 0.112593 -0.000133 39.188 39.212 2.2970
1 1 3 0.114847 0.114825 0.000022 39.619 39.615 2.2730
2 -1 1 0.114880 39.625
1 2 0 0.118362 0.118258 0.000103 40.246 40.228 2.2390
0 1 3 0.118620 40.292
0 0 3 0.127887 0.127836 0.000051 41.907 41.899 2.1540
-2 0 1 0.134806 0.134845 -0.000039 43.081 43.088 2.0980
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 32
M(20)= 36 AV.EPS.= 0.0000514
F 20 = 51.(0.013136, 30)
M(25)= 28 AV.EPS.= 0.0000551
F 25 = 45.(0.012985, 43)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
CHECK IF THERE IS ANY COMMON FACTOR IN THE QUADRATIC FORMS
CHECK CONVERGENCE IN THE REFINEMENT (EV. USE PROGRAM PIRUM OR PURUM)
END OF CALCULATIONS
NUMBER OF CELLS WITH 16 OR MORE INDEXABLE LINES
IN MONOCLINIC (020)-TESTS 0 SOLUTIONS
IN MONOCLINIC SHORT AXIS TESTS 0 SOLUTIONS
IN MONOCLINIC GENERAL TESTS 0 SOLUTIONS
IN TRICLINIC TESTS 25 SOLUTIONS
USED CPU-TIME= 547. SEC.

END OF THE OUTPUT LIST.

COMMENT.

THIS EXAMPLE IS ALSO SHOWN IN THE TREOR90 TEST EXAMPLES BELOW.

THE REDUCED CELL IS OBTAINED BY THE REDUCTION PROGRAM ...REDUCT..
(LOCAL PROGRAM AT UNIV. OF STOCKHOLM. A SIMILAR PROGRAM IS
ALSO ANNOUNCED FROM NBS)
THE OUTPUT LIST FROM REDUCT IS GIVEN BELOW...

*** INPUT CELL ***
A= 5.11754 B= 5.51183 C= 7.03438
ALFA= 73.732 BETA= 73.916 GAMMA= 90.203
TOLERANCE=0.0500

VOLUME OF INPUT CELL= 182.3091 A3

*** REDUCED-CELL ***
A= 5.11754 B= 5.51183 C= 7.03438
ALFA=106.2678 BETA=106.0840 GAMMA= 90.2029

VOLUME OF THE REDUCED CELL= 182.3091 A3

REDUCED FORM NUMBER = 44 INT.TAB.1,SECT. 5.1

*** CONVENTIONAL CELL (METRIC SYMMETRY) ***
TRICLINIC P
A= 5.51183 B= 7.03438 C= 5.11754
ALFA=106.0840 BETA= 90.2029 GAMMA=106.2678

VOLUME OF THE CONVENTIONAL CELL= 182.3091 A3

GENERAL COMMENTS ABOUT THE EXAMPLES GIVEN ABOVE.

1.Data for all examples shown above are taken from National Bureau of Standards (1980). Monograph 25 Section 17.,M.C.Morris, H.F.Mcmurdie, and B.Paretzkin. Standard X-Ray Diffraction Powder Patterns. Sec. 17 Data for 54 substances.

2.In order to reduce the length of the lists above, only examples giving short output lists are chosen. Usually a few more trial cells (with too small De Wolff figure of merit or more than one unindexed line within the first 20 lines) are listed before an acceptable solution is found and the program will stop.

3.The Monograph 25 Section 17 contains

2 Cubic patterns
5 Tetragonal patterns
4 Hexagonal patterns
19 Orthorhombic patterns
18 Monoclinic patterns
6 Triclinic patterns

The following patterns should not be used for TREOR tests..

A. The monoclinic C6H8N2*HCl (p.56), because the B-axis is more than 30 A. As a rule you should be careful if cell edges are more than 20 A. If a cell axis is more than 25 A, synchrotron (or single crystal data) may be needed. For triclinic cells the limit may be about 20 A.
B. The monoclinic NaClO4*H2O (p.68), because the substance is very unstable (as commented im the NBS-report) and the data quality is therefore low. It can only be indexed by TREOR if some special 'tricks' are used (--low De Wolff figure of merit).
C. The triclinic C22H25ClN2OS*2H2O (p.28) because the B-axis is more than 20 A. (See comment A above).
D. The monoclinic CrCl3 (p.23), because it offers some crystallographic non trivial problems. The correct cell (confirmed by single crystal data) is:
A=6.123(2) A, B=10.311(3) A, C=5.956(5) A, BETA=108.64(5) DEG. V= 356.3 A**3 (figures from the NBS monograph).
The M19 reported is 16. A recalculation of the De Wolff figure of merit, taking into account that the unit cell is centered, gives M19=45(which is more convincing). Some other cells, however, will also give acceptable De Wolff figure of merits (---unless density and formula weight is used to exclude the solutions). Following examples may be mentioned:
1. The monoclinic cell
A=11.852(2) A, B=4.664(7) A, C=7.751(3) A, Beta=102.27(2) deg. V=418.6 A**3 and M19=13 (all lines indexed).
2. The triclinic cell. (The found cell was reduced by REDUCT).
A=6.149(2) A, B=7.583(4) A, C=4.871(6) A, Alpha=90.5(2) deg, Beta=104.72(3) deg, Gamma=102.3(2) deg. V=214.2 A**3 and M19=17 (all lines indexed)

All the remaining 50 patterns may be used to test the program..... without using density and formula weights. (It is true that input of density and formula weights will usually considerably reduce CPU-times and make the program more powerful. It is an experience, however, that indexing problems usually have to be solved before any accurate knowledge about composition and density is known.
The monoclinic pattern C4H6Hg2O4 (p.51) is an example where the monoclinic test fails but a correct primitive cell can be found by triclinic test. The triclinic cell is easily reduced to the corrrect monoclinic one by a reduction program (-program REDUCT).

The CPU-times reported above refer to a VAX 11/750.

On CONVEX 210 the CPU-times are about 20-50 times less.

On a PC/AT with math. coprocessor and a 486 CPU computing times are between the CONVEX and the VAX CPU-times.

PC/AT computers with 386 processors may be very time-consuming.

E N D O F TREOR(4)-TEST EXAMPLES

********** ********** **********

T E S T E X A M P L E S U S I N G T R E O R 9 0

O N C O N V E X 2 1 0

********** **********

EXAMPLE 6. INPUT DATA

```
36-431 CU11O2(VO4)6 900119
7.77
7.633
7.528
6.474
5.796
5.423
4.735
4.566
3.941
3.885
3.817
3.639
3.597
3.462
3.309
3.277
3.239
3.187
3.139
3.116
3.091
3.040
3.020
2.898
2.820

CHOICE=4,
VOL=-2000,
END*
```

COMMENT. By using the negative VOL option, all symmetries will be tested.

..... FROM TREOR90 ON THE CONDENSED OUTPUT FILE...

VERSION JANUARY 1990

36-431 CU11O2(VO4)6 900119
7.770000
7.633000
7.528000
6.474000
5.796000
5.423000
4.735000
4.566000
3.941000
3.885000
3.817000
3.639000
3.597000
3.462000
3.309000
3.277000
3.239000
3.187000
3.139000
3.116000
3.091000
3.040000
3.020000
2.898000
2.820000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10
MAX NUMBER OF UNINDEXED LINES IN FIGURE OF MERIT TEST= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 25.0 MAX CELL VOLUME= 2000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
** CUBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** CUBIC TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** TETRAGONAL TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** TETRAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 1000.

SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** MONOCLINIC TEST ********** MAX. VOLUME= 1000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** MONOCLINIC TEST ********** MAX. VOLUME= 2000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** TRICLINIC TEST ********** MAX. VOLUME= 2000.
TRICLINIC DOMINANT ZONE TEST
END OF TRICLINIC DOMINANT ZONE TEST
THIS MAY BE THE SOLUTION !!!
THE REFINEMENT OF THE CELL WILL NOW BE REPEATED
THREE CYCLES MORE. --- GOOD LUCK !

CYCLE RESULTS

0.010470 0.010183 0.009829 0.006163 -0.006497 -0.002349
0.010470 0.010183 0.009829 0.006163 -0.006497 -0.002349
0.010470 0.010183 0.009829 0.006163 -0.006497 -0.002349
NUMBER OF SINGLE INDEXED LINES = 19
TOTAL NUMBER OF LINES = 25
A = 8.268939 0.001039 A ALFA = 88.616623 0.007595 DEG
B = 8.044106 0.000533 A BETA =106.443611 0.008589 DEG
C = 8.157301 0.000479 A GAMMA = 72.854095 0.005014 DEG
UNIT CELL VOLUME = 493.83 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
0 0 1 0.009828 0.009829 -0.000001 11.379 11.380 7.7700
0 1 0 0.010182 0.010183 -0.000001 11.582 11.583 7.6340
1 0 0 0.010470 0.010470 0.000000 11.746 11.746 7.5280
-1 0 1 0.014140 0.014136 0.000003 13.658 13.657 6.4780
1 1 0 0.014156 13.667
0 1 1 0.017663 0.017663 0.000000 15.275 15.275 5.7960
-1 -1 1 0.020176 0.020171 0.000005 16.332 16.330 5.4230
1 0 1 0.026465 0.026463 0.000002 18.725 18.724 4.7350
-1 1 1 0.028461 0.028467 -0.000006 19.425 19.427 4.5660
1 2 0 0.038204 0.038209 -0.000005 22.543 22.544 3.9410
0 0 2 0.039313 0.039318 -0.000005 22.872 22.874 3.8850
-2 0 1 0.039383 22.893
0 2 0 0.040726 0.040732 -0.000006 23.285 23.287 3.8170
0 1 2 0.044808 0.044802 0.000005 24.442 24.440 3.6390
-1 -1 2 0.045845 24.727
0 2 1 0.045860 0.045863 -0.000003 24.731 24.732 3.5970
-1 1 2 0.049443 25.695
1 2 1 0.049507 0.049503 0.000003 25.712 25.711 3.4620
0 -1 2 0.054191 0.054199 -0.000008 26.923 26.925 3.3090
0 -2 1 0.055254 0.055260 -0.000005 27.191 27.192 3.2770
-2 0 2 0.056558 0.056545 0.000014 27.516 27.512 3.2390
2 2 0 0.056626 27.533
-2 -1 2 0.058419 0.058432 -0.000013 27.974 27.977 3.1870
-2 1 1 0.060219 0.060211 0.000009 28.411 28.408 3.1390
1 1 2 0.061112 0.061103 0.000009 28.625 28.623 3.1160
1 0 2 0.062104 0.062115 -0.000010 28.861 28.864 3.0910
2 0 1 0.064037 29.317
-1 2 0 0.064205 0.064196 0.000009 29.356 29.354 3.0400
-2 1 0 0.065059 0.065057 0.000001 29.555 29.555 3.0200
0 2 2 0.070652 0.070653 -0.000002 30.829 30.830 2.8980
-1 -2 2 0.074614 0.074596 0.000018 31.704 31.700 2.8200
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 31
M(20)= 161 AV.EPS.= 0.0000053
F 20 = 366.(0.001519, 36)
M(25)= 145 AV.EPS.= 0.0000059
F 25 = 358.(0.001589, 44)
M CF. J.APPL.CRYST. 1(1968)108

F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
M-TEST= 161 UNINDEXED IN THE TEST= 0

ANY COMMON FACTOR IN THE QUADRATIC FORMS ? ?
CHECK CONVERGENCE IN THE REFINEMENT
(EV. USE PROGRAM PIRUM OR PURUM)
END OF INDEXING CALCULATIONS

The following unit cell reduction is ONLY valid if,
and ONLY IF the unit cell found is PRIMITIVE.
If the unit cell found is not primitive, you have to
convert the cell to a primitive one and run a cell
reduction program separately.

*** INPUT CELL ***
A= 8.26894 B= 8.04411 C= 8.15730
ALFA= 88.617 BETA=106.444 GAMMA= 72.854
TOLERANCE=0.0500

VOLUME OF INPUT CELL= 493.83 A3

*** REDUCED-CELL ***
A= 8.04411 B= 8.15730 C= 8.26894
ALFA=106.4437 BETA=107.1459 GAMMA= 91.3834

VOLUME OF THE REDUCED CELL= 493.83 A3

REDUCED FORM NUMBER = 44 INT.TAB.1,SECT. 5.1

*** CONVENTIONAL CELL (METRIC SYMMETRY) ***
TRICLINIC P
A= 8.15730 B= 8.26894 C= 8.04411
ALFA=107.1459 BETA= 91.3834 GAMMA=106.4437

VOLUME OF THE CONVENTIONAL CELL= 493.83 A3

IF YOU WANT TO LOOK FOR A BETTER SOLUTION YOU
MAY TRY TO INCREASE THE PARAMETER MERIT ABOVE 161
....OR PERHAPS THIS WAS THE BEST SOLUTION...
USED CPU-TIME= 50.00 SEC.

END OF THE CONDENSED OUTPUT LIST.
COMMENT.
As seen above the program ends with a cell reduction routine.
Note that volume limits are changed by statistical methods during
the treor run. Therefore, the user does not need to worry much
about possible unit cell volumes.

EXAMPLE 7. INPUT DATA

NBS.25 SEC.17 P.64 K2S2O8
5.27
4.892
4.847
4.602
3.750
3.699
3.603
3.443
3.268
3.232
3.153
3.025
2.736
2.634
2.548
2.466
2.419
2.397
2.358
2.315
2.297
2.273
2.239
2.154
2.098

CHOICE=4,
VOL=-2000,
END*

COMMENT. Compare this example with no.5 above. It is the same pattern runned with TREOR90. It is a normal run, wich means that it starts with cubic symmmetry etc.

.....FROM TREOR90 ON THE CONDENSED OUTPUT FILE...

VERSION JANUARY 1990
NBS.25 SEC.17 P.64 K2S2O8
5.270000
4.892000
4.847000
4.602000
3.750000
3.699000
3.603000
3.443000
3.268000
3.232000
3.153000
3.025000

2.736000
2.634000
2.548000
2.466000
2.419000
2.397000
2.358000
2.315000
2.297000
2.273000
2.239000
2.154000
2.098000
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10
MAX NUMBER OF UNINDEXED LINES IN FIGURE OF MERIT TEST= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 25.0 MAX CELL VOLUME= 2000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
** CUBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** CUBIC TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** TETRAGONAL TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** TETRAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 2000.

SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** MONOCLINIC TEST ********** MAX. VOLUME= 1000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** MONOCLINIC TEST ********** MAX. VOLUME= 2000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** TRICLINIC TEST ********** MAX. VOLUME= 2000.
TRICLINIC DOMINANT ZONE TEST
END OF TRICLINIC DOMINANT ZONE TEST
THIS MAY BE THE SOLUTION !!!
THE REFINEMENT OF THE CELL WILL NOW BE REPEATED
THREE CYCLES MORE. --- GOOD LUCK !

CYCLE RESULTS

0.024732 0.021360 0.014204 -0.010857 0.004044 -0.010192
0.024732 0.021360 0.014204 -0.010857 0.004044 -0.010192
0.024732 0.021360 0.014204 -0.010857 0.004044 -0.010192
NUMBER OF SINGLE INDEXED LINES = 19
TOTAL NUMBER OF LINES = 25
A = 5.117540 0.001495 A ALFA = 73.732155 0.028466 DEG
B = 5.511827 0.002494 A BETA = 73.916039 0.040241 DEG
C = 7.034379 0.002352 A GAMMA = 90.202797 0.030144 DEG
UNIT CELL VOLUME = 182.31 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
0 1 0 0.021381 0.021360 0.000021 16.816 16.808 5.2680

1 0 0 0.024794 0.024732 0.000062 18.119 18.096 4.8920
0 1 1 0.025351 0.025372 -0.000021 18.323 18.331 4.8380
1 0 1 0.028115 0.028079 0.000036 19.305 19.293 4.5940
-1 1 0 0.042195 0.042047 0.000147 23.707 23.665 3.7500
1 1 1 0.043366 0.043290 0.000076 24.039 24.018 3.6990
0 -1 1 0.045708 0.045755 -0.000048 24.690 24.703 3.6030
1 1 0 0.050055 0.050135 -0.000081 25.856 25.878 3.4430
1 -1 1 0.055559 0.055586 -0.000027 27.267 27.274 3.2680
0 0 2 0.056804 0.056816 -0.000012 27.577 27.580 3.2320
-1 1 1 0.056917 27.605
1 0 2 0.059686 0.059833 -0.000148 28.282 28.317 3.1530
1 1 2 0.064844 0.064854 -0.000010 29.505 29.507 3.0250
0 2 1 0.079266 0.079259 0.000007 32.705 32.703 2.7360
-1 -1 1 0.085388 33.981
0 2 0 0.085524 0.085438 0.000085 34.009 33.991 2.6340
2 0 1 0.091394 0.091416 -0.000022 35.193 35.198 2.5480
1 -1 2 0.097574 0.097533 0.000041 36.404 36.396 2.4660
1 2 1 0.101222 37.103
0 2 2 0.101402 0.101487 -0.000085 37.137 37.153 2.4190
-1 0 2 0.103272 0.103262 0.000010 37.490 37.488 2.3970
-1 2 1 0.106716 0.106759 -0.000043 38.134 38.142 2.3580
2 1 1 0.110718 0.110672 0.000045 38.871 38.862 2.3150
-2 1 0 0.112198 39.140
2 0 2 0.112314 39.161
1 2 2 0.112460 0.112593 -0.000133 39.188 39.212 2.2970
1 1 3 0.114847 0.114825 0.000022 39.619 39.615 2.2730
2 -1 1 0.114880 39.625
1 2 0 0.118362 0.118258 0.000103 40.246 40.228 2.2390
0 1 3 0.118620 40.292
0 0 3 0.127887 0.127836 0.000051 41.907 41.899 2.1540
-2 0 1 0.134806 0.134845 -0.000039 43.081 43.088 2.0980
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 32
M(20)= 36 AV.EPS.= 0.0000514
F 20 = 51.(0.013134, 30)
M(25)= 28 AV.EPS.= 0.0000551
F 25 = 45.(0.012984, 43)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
M-TEST= 36 UNINDEXED IN THE TEST= 0

ANY COMMON FACTOR IN THE QUADRATIC FORMS ? ?
CHECK CONVERGENCE IN THE REFINEMENT
(EV. USE PROGRAM PIRUM OR PURUM)
END OF INDEXING CALCULATIONS

The following unit cell reduction is ONLY valid if,
and ONLY IF the unit cell found is PRIMITIVE.

If the unit cell found is not primitive, you have to
convert the cell to a primitive one and run a cell
reduction program separately.

*** INPUT CELL ***
A= 5.11754 B= 5.51183 C= 7.03438
ALFA= 73.732 BETA= 73.916 GAMMA= 90.203
TOLERANCE=0.0500

VOLUME OF INPUT CELL= 182.31 A3

*** REDUCED-CELL ***
A= 5.11754 B= 5.51183 C= 7.03438
ALFA=106.2678 BETA=106.0840 GAMMA= 90.2029

VOLUME OF THE REDUCED CELL= 182.31 A3

REDUCED FORM NUMBER = 44 INT.TAB.1,SECT. 5.1

*** CONVENTIONAL CELL (METRIC SYMMETRY) ***
TRICLINIC P
A= 5.51183 B= 7.03438 C= 5.11754
ALFA=106.0840 BETA= 90.2029 GAMMA=106.2678

VOLUME OF THE CONVENTIONAL CELL= 182.31 A3

IF YOU WANT TO LOOK FOR A BETTER SOLUTION YOU
MAY TRY TO INCREASE THE PARAMETER MERIT ABOVE 36
....OR PERHAPS THIS WAS THE BEST SOLUTION...
USED CPU-TIME= 131.00 SEC.

COMMENT. For the triclinic part of this run the used CPU-time
46 sec. The time is rather long because the normal
max. volume input was used. (VOL=-2000)
The user did not need to estimate a reasonable volume.

Note also that the general output lists have not been
printed here. The user will be informed (on the display)
if an interesting result has been obtained and will be
asked to not print the sometimes very long general
output lists.

EXAMPLE 8. INPUT DATA

TRICLINIC TEST 25.16 P.92 280889
15.83 40
8.75 60
7.91 4
7.78 13
7.56 14
7.03 8
6.67 39

```
6.21 3
5.77 48
5.53 100
5.29 14
5.02 2
4.96 1
4.85 4
4.52 2
4.454 7
4.410 7
4.312 24
4.263 10
4.184 2
4.081 4
4.044 1
3.962 3
3.890 3
3.844 8

CHOICE=4,
VOL=-2000,
END*
```

COMMENT. In this example also the intensities are given.
They are never used in the calculations, but are
printed on the output lists.

.....FROM TREOR90 ON THE CONDENSED OUTPUT FILE.....

```
VERSION JANUARY 1990
TRICLINIC TEST 25.16 P.92 280889
15.830000 40
8.750000 60
7.910000 4
7.780000 13
7.560000 14
7.030000 8
6.670000 39
6.210000 3
5.770000 48
5.530000 100
5.290000 14
5.020000 2
4.960000 1
4.850000 4
4.520000 2
4.454000 7
4.410000 7
4.312000 24
4.263000 10
```

4.184000 2
4.081000 4
4.044000 1
3.962000 3
3.890000 3
3.844000 8
LINE NUMBER= 3 SHOULD NOT BE INCLUDED IN THE TREOR
BASE LINE SETS. SINE SQUARE THETA FOR THIS LINE = 4
TIMES SINE SQUARE THETA FOR LINE NUMBER = 1
---LINE NUMBER= 3 WILL BE SKIPPED IN THE TRIAL PHASE.
STOP LIMITS
FIGURE OF MERIT REQUIRED= 10
MAX NUMBER OF UNINDEXED LINES IN FIGURE OF MERIT TEST= 1
THE 7 FIRST LINES ADJUSTED BY THEIR HIGHER ORDERS
CUBIC,TETRAGONAL,HEXAGONAL AND ORTHOROMBIC SYMMETRY
MAX CELL EDGE= 25.0 MAX CELL VOLUME= 2000.0
D1= 0.000200 SSQTL= 0.050000 D2= 0.000400 WAVE= 1.540598
NUMBER OF TEST LINES= 19 IQ REQUIRED= 16
** CUBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** CUBIC TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1) (2)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 6
** TETRAGONAL TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** TETRAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** HEXAGONAL TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2) (1,3) (2,3)
BASE LINE ONE.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
BASE LINE TWO.(HKL)-MAX= 4 4 4 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 1000.
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** ORTHORHOMBIC TEST ********** MAX. VOLUME= 2000.
SELECTED BASE LINES (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 4

BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
** MONOCLINIC TEST ********** MAX. VOLUME= 1000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** MONOCLINIC TEST ********** MAX. VOLUME= 2000.
MAX BETA ALLOWED= 135 DEG.
(020)-SEARCH
SELECTED BASE LINES (1,2,3,4) (1,2,3,5) (1,2,4,5)
BASE LINE ONE.(HKL)-MAX= 2 2 2 MAX H+K+L= 2
BASE LINE TWO.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE THREE.(HKL)-MAX= 2 2 2 MAX H+K+L= 3
BASE LINE FOUR.(HKL)-MAX= 2 2 2 MAX H+K+L= 4
SELECTED BASE LINES= 1 3 4 5
SELECTED BASE LINES= 1 2 3 6
SELECTED BASE LINES= 2 3 4 5
SELECTED BASE LINES= 1 2 3 7
** TRICLINIC TEST ********** MAX. VOLUME= 2000.
TRICLINIC DOMINANT ZONE TEST
THIS MAY BE THE SOLUTION !!!
THE REFINEMENT OF THE CELL WILL NOW BE REPEATED
THREE CYCLES MORE. --- GOOD LUCK !

CYCLE RESULTS

0.011991 0.009791 0.002362 -0.001026 0.002341 -0.004419
0.011991 0.009791 0.002362 -0.001026 0.002341 -0.004419
0.011991 0.009791 0.002362 -0.001026 0.002341 -0.004419
NUMBER OF SINGLE INDEXED LINES = 22
TOTAL NUMBER OF LINES = 25
A = 7.085807 0.003240 A ALFA = 63.013237 0.035016 DEG
B = 8.787556 0.003735 A BETA = 86.963554 0.076038 DEG
C = 17.870726 0.009100 A GAMMA = 94.134857 0.035155 DEG
UNIT CELL VOLUME = 984.40 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
0 0 1 0.002362 0.002362 0.000001 5.572 5.571 15.8480 40
0 1 1 0.007750 0.007734 0.000016 10.101 10.091 8.7500 60
0 0 2 0.009450 0.009447 0.000003 11.157 11.155 7.9240 4
0 1 0 0.009803 0.009791 0.000012 11.364 11.357 7.7800 13
0 1 2 0.010382 0.010400 -0.000019 11.696 11.707 7.5600 14

1 0 0 0.012006 0.011991 0.000015 12.581 12.573 7.0300 8
1 0 1 0.013337 0.013327 0.000011 13.263 13.258 6.6700 39
-1 0 1 0.015386 0.015379 0.000007 14.251 14.247 6.2100 3
0 1 3 0.017822 0.017790 0.000032 15.344 15.330 5.7700 48
1 0 2 0.019403 0.019386 0.000017 16.014 16.007 5.5300 100
-1 1 0 0.019441 16.030
1 1 1 0.021040 16.681
0 0 3 0.021203 0.021255 -0.000052 16.746 16.766 5.2900 14
-1 0 2 0.023546 0.023490 0.000055 17.653 17.632 5.0200 2
1 1 0 0.024119 0.024123 -0.000004 17.869 17.870 4.9600 1
1 -1 1 0.025225 0.025195 0.000030 18.277 18.266 4.8500 4
1 1 3 0.029043 0.029044 -0.000001 19.624 19.625 4.5200 2
0 1 4 0.029910 0.029904 0.000006 19.918 19.916 4.4540 7
-1 1 3 0.030510 0.030519 -0.000009 20.119 20.122 4.4100 7
-1 -1 1 0.031913 0.031930 -0.000017 20.581 20.587 4.3120 24
0 2 1 0.032650 0.032688 -0.000037 20.820 20.832 4.2630 10
0 2 3 0.033895 0.033907 -0.000012 21.218 21.222 4.1840 2
1 -1 2 0.035628 0.035672 -0.000045 21.760 21.774 4.0810 4
-1 0 3 0.036282 0.036325 -0.000043 21.962 21.975 4.0440 1
0 0 4 0.037800 0.037787 0.000012 22.422 22.418 3.9620 3
0 2 0 0.039212 0.039163 0.000049 22.842 22.828 3.8900 3
1 1 4 0.040156 0.040132 0.000025 23.120 23.112 3.8440 8
-1 2 2 0.040296 23.160
NUMBER OF OBS. LINES = 25
NUMBER OF CALC. LINES = 28
M(20)= 34 AV.EPS.= 0.0000179
F 20 = 96.(0.007500, 28)
M(25)= 28 AV.EPS.= 0.0000213
F 25 = 91.(0.008089, 34)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60
0 LINES ARE UNINDEXED
M-TEST= 34 UNINDEXED IN THE TEST= 0

ANY COMMON FACTOR IN THE QUADRATIC FORMS ? ?
CHECK CONVERGENCE IN THE REFINEMENT
(EV. USE PROGRAM PIRUM OR PURUM)
END OF INDEXING CALCULATIONS

The following unit cell reduction is ONLY valid if,
and ONLY IF the unit cell found is PRIMITIVE.
If the unit cell found is not primitive, you have to
convert the cell to a primitive one and run a cell
reduction program separately.

*** INPUT CELL ***
A= 7.08581 B= 8.78756 C= 17.87073
ALFA= 63.013 BETA= 86.964 GAMMA= 94.135
TOLERANCE=0.0500

VOLUME OF INPUT CELL= 984.40 A3

*** REDUCED-CELL ***
A= 7.08581 B= 8.78756 C= 15.93924
ALFA= 87.5617 BETA= 84.3102 GAMMA= 85.8651

VOLUME OF THE REDUCED CELL= 984.40 A3

REDUCED FORM NUMBER = 31 INT.TAB.1,SECT. 5.1

*** CONVENTIONAL CELL (METRIC SYMMETRY) ***
TRICLINIC P
A= 8.78756 B= 15.93924 C= 7.08581
ALFA= 95.6898 BETA= 94.1349 GAMMA= 87.5617

VOLUME OF THE CONVENTIONAL CELL= 984.40 A3

IF YOU WANT TO LOOK FOR A BETTER SOLUTION YOU
MAY TRY TO INCREASE THE PARAMETER MERIT ABOVE 34
....OR PERHAPS THIS WAS THE BEST SOLUTION...
USED CPU-TIME= 30.00 SEC.

COMMENT. This is a typical dominant zone example. As can be seen
on the output list the first 5 lines have h=0. Note that
TREOR90 automatically deletes line no.3 from the base
line sets because it is within error limits 1/2 of the
first line, i.e. it does not contain information about
any new parameter.It is included in the final refinement
and output list, however. In earlier TREOR versions the
user had to exclude such lines from the input data.

********** ********** **********
All examples discussed above are easily solved and automatically
confirmed by a run going through all symmetries in TREOR97 mode.

Title line.
Data lines
Blank line
choice=4, end* (may be written in lower case on one line)

Below is the condensed output list from Example 3 using the TREOR97 mode.

Version: September 1997
Example 3. NBS.25 SEC.17 P.9 (NH4)2NI(SO4)2*6H2O
7.190000
6.240000
5.980000
5.388000
5.248000
5.090000
4.397000
4.316000

4.243000
4.166000
4.147000
3.952000
3.757000
3.586000
3.466000
3.410000
3.376000
3.119000
3.037000
3.027000
2.943000
2.913000
2.903000
2.892000
2.853000
TREOR97 mode.
Stop limits
Figure of merit required= 10
Max number of unindexed lines in figure of merit test= 1
The 7 first lines adjusted by their higher orders
Max cell edge= 25.0 Max cell volume= 2000.0
D1= .000200 SSQTL= .050000 D2= .000400 WAVE= 1.540598
Number of test lines= 19 IQ required= 16
** CUBIC test ********** Max. volume= 1000.
Selected base lines (1) (2)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 6
** CUBIC test ********** Max. volume= 2000.
Selected base lines (1) (2)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 6
** TETRAGONAL test ********** Max. volume= 1000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** TETRAGONAL test ********** Max. volume= 2000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** HEXAGONAL test ********** Max. volume= 1000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** HEXAGONAL test ********** Max. volume= 2000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** ORTHORHOMBIC test ********** Max. volume= 1000.
Selected base lines (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)

Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 4
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 4
** ORTHORHOMBIC test ********** Max. volume= 2000.
Selected base lines (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 4
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 4
** MONOCLINIC test ********** Max. volume= 1000.
Max beta allowed= 135 deg.
(020)-search
This may be the solution !!!
Refinement of the cell will now be repeated
three cycles more. --- !

Cycle results

.007679 .003814 .016640 .006579 .000000 .000000
.007679 .003814 .016640 .006579 .000000 .000000
.007679 .003814 .016640 .006579 .000000 .000000
Number of single indexed lines = 20
Total number of lines = 25
A = 9.188087 .001842 A alpha = 90.000000 .000000 deg
B = 12.472350 .004108 A beta =106.917400 .020981 deg
C = 6.241650 .001464 A gamma = 90.000000 .000000 deg
Unit cell volume = 684.32 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
1 1 0 .011478 .011493 -.000015 12.300 12.309 7.1900
0 2 0 .015249 .015257 -.000009 14.187 14.191 6.2380
0 0 1 .016593 .016640 -.000047 14.802 14.823 5.9800
0 1 1 .020439 .020454 -.000015 16.439 16.445 5.3880
-1 1 1 .021544 .021554 -.000010 16.881 16.885 5.2480
1 2 0 .022903 .022936 -.000034 17.409 17.422 5.0900
2 0 0 .030691 .030715 -.000025 20.179 20.187 4.3970
0 2 1 .031853 .031897 -.000044 20.562 20.576 4.3160
-1 2 1 .032959 .032997 -.000039 20.920 20.932 4.2430
-2 0 1 .034189 .034198 -.000009 21.311 21.314 4.1660
0 3 0 .034329 21.355
2 1 0 .034503 .034530 -.000027 21.410 21.418 4.1470
-2 1 1 .037991 .038012 -.000021 22.479 22.486 3.9520
1 3 0 .042037 .042008 .000029 23.663 23.654 3.7570
2 2 0 .045973 24.762
1 2 1 .046142 .046154 -.000012 24.808 24.812 3.5860
-2 2 1 .049393 .049455 -.000063 25.682 25.698 3.4660
0 3 1 .051028 .050969 .000059 26.111 26.096 3.4100
-1 3 1 .052061 .052069 -.000008 26.379 26.381 3.3760
0 4 0 .060994 .061030 -.000036 28.597 28.605 3.1190
-1 0 2 .061080 28.617

2 1 1 .064332 .064326 .000006 29.386 29.384 3.0370
-1 1 2 .064758 .064895 -.000137 29.485 29.517 3.0270
2 3 0 .065044 29.552
-2 3 1 .068508 .068527 -.000020 30.347 30.351 2.9430
1 4 0 .068709 30.392
-3 1 1 .069926 .069828 .000098 30.667 30.645 2.9130
0 1 2 .070408 .070373 .000035 30.775 30.767 2.9030
-2 0 2 .070945 .070960 -.000015 30.895 30.898 2.8920
3 1 0 .072898 .072924 -.000026 31.328 31.334 2.8530
Number of OBS. lines = 25
Number of CALC. lines = 30
M(20)= 36 AV.EPS.= .0000322
F 20 = 73.(.009821, 28)
M(25)= 28 AV.EPS.= .0000335
F 25 = 67.(.009591, 39)
M cf. J.Appl.Crystallogr. 1(1968)108
F cf. J.Appl.Crystallogr. 12(1979)60
0 Lines are unindexed
M-test= 36 Unindexed in the test= 0

Any common factor in the quadratic forms ? ?
Check convergence in the refinement
(cf. Program PIRUM)

The following unit cell reduction is ONLY valid if,
and ONLY IF the unit cell found is PRIMITIVE.
If the unit cell found is not primitive, you have to
convert the cell to a primitive one and run a cell
reduction program separately.

*** Input cell ***
A= 9.18809 B= 12.47235 C= 6.24165
ALFA= 90.000 BETA=106.917 GAMMA= 90.000
TOLERANCE= .0500

Volume of input cell= 684.32 A3

*** Reduced cell ***
A= 6.24165 B= 9.18809 C= 12.47235
ALFA= 90.0000 BETA= 90.0000 GAMMA=106.9175

Volume of the reduced cell= 684.32 A3

Reduced form number = 34 Int.TAB.1,Sect. 5.1

*** Conventional cell (Metric symmetry) ***
Monoclinic P
A= 9.18809 B= 12.47235 C= 6.24165
ALFA= 90.0000 BETA=106.9175 GAMMA= 90.0000

Volume of the conventional cell= 684.32 A3

If you want to look for a better solution you
may try to increase the parameter MERIT above 36
....or perhaps this was the best solution...
Version: September 1997
Example 3. NBS.25 SEC.17 P.9 (NH4)2NI(SO4)2*6H2O
7.190000
6.240000
5.980000
5.388000
5.248000
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4.147000
3.952000
3.757000
3.586000
3.466000
3.410000
3.376000
3.119000
3.037000
3.027000
2.943000
2.913000
2.903000
2.892000
2.853000
TREOR97 mode.
Stop limits
Figure of merit required= 37
Max number of unindexed lines in figure of merit test= 1
The 7 first lines adjusted by their higher orders
Max cell edge= 25.0 Max cell volume= 2000.0
D1= .000200 SSQTL= .050000 D2= .000400 WAVE= 1.540598
Number of test lines= 19 IQ required= 16
** CUBIC test ********** Max. volume= 1000.
Selected base lines (1) (2)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 6
** CUBIC test ********** Max. volume= 2000.
Selected base lines (1) (2)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 6
** TETRAGONAL test ********** Max. volume= 1000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** TETRAGONAL test ********** Max. volume= 2000.

Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** HEXAGONAL test ********** Max. volume= 1000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** HEXAGONAL test ********** Max. volume= 2000.
Selected base lines (1,2) (1,3) (2,3)
Base line one.(HKL)-Max= 4 4 4 Max H+K+L= 4
Base line two.(HKL)-Max= 4 4 4 Max H+K+L= 4
** ORTHORHOMBIC test ********** Max. volume= 1000.
Selected base lines (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 4
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 4
** ORTHORHOMBIC test ********** Max. volume= 2000.
Selected base lines (1,2,3) (1,2,4) (1,2,5) (1,3,4) (2,3,4) (1,2,6)
Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 4
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 4
** MONOCLINIC test ********** Max. volume= 1000.
Max beta allowed= 135 deg.
(020)-search
Selected base lines (1,2,3,4) (1,2,3,5) (1,2,4,5)
Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 2
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line four.(HKL)-Max= 2 2 2 Max H+K+L= 4
Selected base lines= 1 3 4 5
Selected base lines= 1 2 3 6
Selected base lines= 2 3 4 5
Selected base lines= 1 2 3 7
** MONOCLINIC test ********** Max. volume= 2000.
Max beta allowed= 135 deg.
(020)-search
Selected base lines (1,2,3,4) (1,2,3,5) (1,2,4,5)
Base line one.(HKL)-Max= 2 2 2 Max H+K+L= 2
Base line two.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line three.(HKL)-Max= 2 2 2 Max H+K+L= 3
Base line four.(HKL)-Max= 2 2 2 Max H+K+L= 4
Selected base lines= 1 3 4 5
Selected base lines= 1 2 3 6
Selected base lines= 2 3 4 5
Selected base lines= 1 2 3 7
Number of plausible solutions = 1

..... E N D.....E N D.....E N D.....E N D.....