SINGLE2010
Users manual

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INTRODUCTION

SINGLE is a program maintained and developed by RJ Angel to carry out the calculations necessary for controlling a four-circle Eulerian-cradle diffractometer. It is developed from earlier versions of SINGLE written by LW Finger (Geophysical Laboratory, CIW) and RJ Angel. Much of the code is derived from software written earlier by LW Finger.

The software is currently supplied on a non-commercial basis. The author would therefore appreciate acknowledgement of the use of the code being made in all publications that make use of data collected or processed using SINGLE. Relevant literature is:

> The SINGLE code itself and many of the algorithms used - Angel RJ, Finger LW (2011) SINGLE: a program to control single-crystal diffractometers. *J. Appl. Cryst.,* 44:247-251.
>
> The peak centering algorithms are described in Angel et al., *J. Appl. Cryst.,* 30:461-466 (1997).
>
> The method of diffracted beam centering (otherwise known as 8-position centering) used in the ZREF utility was originally developed by Hamilton. The practical implementation was first described by King and Finger, *J. Appl. Cryst.,* 12:374-378 (1979).
>
> The method of constrained vector least-squares to obtain cell parameters in the CLSQ utility was developed by Ralph and Finger, *J. Appl. Cryst.,* 15:537-539 (1982).

While the authors are pleased to receive reports of bugs in the code and suggestions for changes and improvements, the authors take no responsibility for any incorrect operation of the code. The authors accept no liability for damage caused through use of this code to control equipment.

1. VERSION NOTES

Single2010 can run under Windows-98, Windows-XP, and 32-bit and 64-bit Windows-7. It has not been used under Vista, or NT. It does not work under Windows-2000.

The current version of the code is **Single2010**. It was originally established in summer 2010 as the final version of Single2008 which was developed over the previous two years. Single2008 was created from the previous release Single04 in Spring 2008, and installed and tested in Bayreuth and Virginia Tech Crystallography Laboratory (VTX) in the period May-June 2008, further modified and tested at Padua, BGI, Heidelberg and VTX in fall 2008, and VTX, BGI, Padua in Summer 2009. The P4 interface was developed in Innsbruck in September 2009-May 2010, and the interface for the SMC9300 was developed at the same time in Bayreuth.

Significant changes in **Single2010** from **Single04**, included:

- Restructuring of code to separate diffractometer-dependent code from the communications subroutines. Standardisation of the diffractometer-dependent code so allows easier implementation of new diffractometer interfaces.
- Implementation of interfaces for Stoe Stadi4, Siemens P4 and Huber SMC9300.
- Support for both Windows-98 and Windows-XP communications via serial ports or USB/Serial adaptors.
- More traps of communication errors, and more recovery routines.
- Support for choice of line terminators via the *difprof.dat* file.
- Reduction of interface calls by keeping a log of motor positions.
- Generalisation of motor names, to make internal motor numbers always to correspond to 1 = 2θ, 2 = ω(bisecting), 3 = χ, 4 = ϕ, 5 = vertical slits, 6 = horizontal slits. Local translation of motor names to these numbers is via entries in the *difprof.dat* file.
- Introduction of motor numbers 7 = detector drive, 8 = sample height.
- If motorised slits are not present, the slit settings can be loaded with the **ldmt** command.
- Introduction of a *STOP* button.
- Introduction of ZREM command to do zref on multiple crystals from one command, and CEN8 command to do 8-position centering on one reflection.
- Introduction of the INL command to input reflection indices in to the list by Laue group.
- Re-introduction of SRCH and CONE searches.
- Program is distributed as one *exe* file. Choice of diffractometer done via *difprof.dat*

Further changes to commands in **Single2010** from May 2010 to March 2012 include:

- Re-introduction of PHOT and CALP to do rotation photographs.
- Introduction of UBIM and UBEX commands to import and export UB matrices. These replace the previous OMX command.
- Introduction of STEP command to perform step scan of any diffractometer circle with the shutter closed.
- Intensity data collection commands have been renamed:
    - INTA to DC S
    - INTL to DC L
    - INTS to DC I
    - PSI to DC P
- The CALC command can now report 8 positions.
- The SORT command can now sort on all items in the list, not just 2theta
- Introduction of the MACR command to run a list of commands stored in a text file.
- Introduction of the FREF command to initiate a search for circle reference points on the Stadi4.

- The refinement of trigonal unit-cells was added to **clsq** and **tlsq**.
- The telescope message is now controller-dependent so that it does not appear on the P4.
- More information is provided after a failure in centering.
- Additional parameters have been introduced for working with high-temperature furnaces.
- More information about the program version and configuration is written to the user log file when the program starts.

For details of the new and changed commands, please read the section on COMMANDS in the user manual.

There have also been a number of developments in the code, and changes to controllers, in order to improve the precision of the unit-cell parameters determined by the ZREF procedure:

- When motor steps are not exact multiples of 0.001^{o}, correct operation requires that the Huber SMC9300 motor controller is set to report positions to 4 decimal places. See the section in this manual on the SMC9300 controller.
- The fitting of omega peak profiles collected on instruments fitted with a monochromator was corrected.
- The angular positions are now written in to the *rfl* file with additional decimal places to accommodate motor steps that are not exact multiples of 0.001^{o}.

In combination with changes to the separate Zref and WinIntegrStp programs, these code changes and changes to the SMC9300 controller configuration means that the unit-cells obtained by fitting data with these programs is identical to the results from LSQ and CLSQ in Single.

2. GENERAL PRINCIPLES

The program is written to be mainly diffractometer-independent. It can also be run without a diffractometer attached. This option can be selected by the user upon starting the program, and is indicated by the command line prompt of the program including the string "DMSINGLE".

The circle conventions and parities, and axial systems of Busing and Levy (1967) are used for all calculations. When all circles are at their zero positions:

- the 2θ arm lies in the position of the undiffracted direct beam ($2\theta = 0$),
- the plane of the χ circle is perpendicular to the direct beam ($\omega = 0$),
- the ϕ axis is perpendicular to the diffraction plane ($\chi = 0$),
- the choice of $\phi = 0$ is arbitrary.

These conventions also define the "normal-beam equatorial geometry" of Arndt and Willis (1966) subsequently generalised by Dera and Katrusiak (1998). In these zero positions the Cartesian basis of the “ϕ axis” coordinate system (Busing and Levy 1967) has its axes defined as follows:

- the origin is at the centre of the diffractometer,
- the positive *y* axis extends from the crystal towards the detector (i.e. along the undiffracted direct beam),
- the positive *z* axis is parallel to the ϕ axis, perpendicular to the diffraction plane, and away from the ϕ axis carrier,
- the positive *x* axis makes a right-handed set, and corresponds to an imaginary diffraction vector at $2\theta = 0$.

The sense of positive rotations of the four diffractometer circles under the Busing and Levy

(1967) convention are left-handed for all axes except for the χ axis. To be explicit, when viewed *from the +z direction* (looking down on the diffractometer from above), positive movement of the 2θ, ω and ϕ axes away from their zero positions is clockwise. When viewed *from the +y direction* (looking towards the crystal from the detector arm) positive movement of the χ axis is anti-clockwise. These senses of rotations are defined as having *positive parities*.

The user interface always refers to the circles and slits by the same numbers, independent of the diffractometer controller; 1 = 2θ, 2 = ω(bisecting), 3 = χ, 4 = ϕ, 5 = vertical slits, 6 = horizontal slits, 7 = detector drive, 8 = sample height. Local translation of these numbers to actual motor names used by the diffractometer interface or controller is set by entries in the *difprof.dat* file.

2.1. Files

The SINGLE software uses several files. They are all Ascii files that can be read by any text editor such as Notepad or Wordpad. They can become corrupted if opened with a utility such as Word.

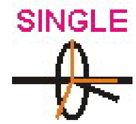
The files are:

1. **difprof.dat**. Holds two types of information. First, diffractometer-dependent parameters such as motor drive information. Further details of these parameters are given in the installation guide. They should not normally be changed. The *difprof.dat* file also contains default parameters for centering scans and for data collections. These parameters are only used when a new mat file is created at start-up of the SINGLE software. *Difprof.dat* must reside in the same directory as the SINGLE executable.
2. **single.log**. The instrument log file. Resides in the same directory as the SINGLE executable. Created by SINGLE. Holds any warning or error messages generated by the program. Do not edit as it provides a permanent record of instrument errors.
3. **mat file**. Contains all of the information related to the individual experiment on one crystal, including the experiment title, the UB matrix, wavelength and scan parameters, the indices, setting angles and intensities of reflections used in centering, data collection parameters. The file name extension must always be “.mat”. The file can reside anywhere, but best not with the SINGLE executable.

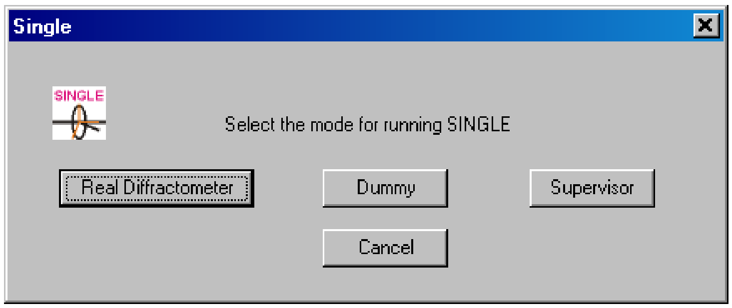
   Note: If an old matfile is opened (at start-up or later) all of the scan parameters etc are loaded from the file. If a new matfile is created when starting the SINGLE program, the parameters are loaded immediately from the values in *difprof.dat*. If a new matfile is created with the set matfile command, then all of the current parameters are written to the new file, *not* the ones in *difprof.dat*. The matfile is immediately re-written with the current parameters whenever the parameters or peak list information is changed (e.g. upon centering).
4. **User log file**. Created by SINGLE, and given the same name as the *mat* file but with the extension *.log*. Resides in the same directory as the mat file. All of the information on the terminal screen (input and output) is copied to this file as a permanent record of the experiment. Can be examined while the program is running, or afterwards, by a text editor such as Wordpad.
5. **Centering scans file**. Created by SINGLE, and given the same name as the *mat* file with “_cntr.rfl” added. Resides in the same directory as the mat file. It is a standard-format reflection file containing the step-scan data of the final ω scans from centering with the **zref** command, and also other ω scans if **log** is activated. Can be used by WinIntegrStp to examine and refit the profiles after the experiment.
6. **Data collection file**. Created by user with the **set datfile** command. Can reside anywhere. It is a standard-format reflection file containing the step-scan data collected during a data

collection.
7. **Reflection list file**. Created by user with a text editor. Can reside anywhere. Contains a list of reflection indices, one reflection per line, to be collected with the **dc l** command.

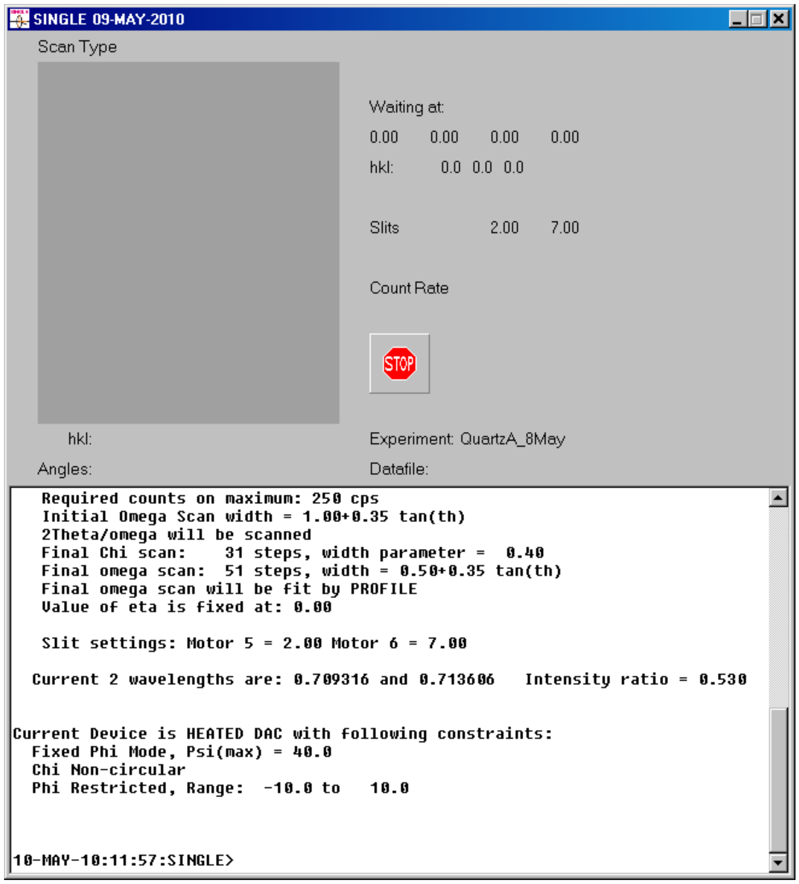
3. RUNNING THE PROGRAM WITH THE DIFFRACTOMETER

1. Double-click on the SINGLE shortcut on the desktop: 

2. A dialog box will appear:



3. In the dialog box, select “Real Diffractometer”. If the installation is ok the main window will appear. In the scrolling region of the window, the following messages will appear in order:
    a. The Version information.
    b. OPENING COMMUNICATIONS ON COM**n** ....please wait ”
        i. If this does not appear, you have a windows system problem.
        ii. If nothing else appears, or you get an error message, then either the parameters in *difprof.dat* are wrong, or your diffractometer controller is not responding. Exit the program and check both.
    c. “Checking motor positions, please wait:”
        i. For each motor you should see either “OK”
        ii. or a message to say that the stored position in the controller does not match the park position
        iii. or some other error message. Correct the problem and restart the program.
4. Then the motor positions will be updated on the display, and a file browser will appear:
    a. Use the browser to select your data directory.
    b. Type in the name for the experiment (“mat”) file. Do not use an extension.
5. The program should now load some default parameters and the window should look something like this:



The program is now ready for your commands (see section below).

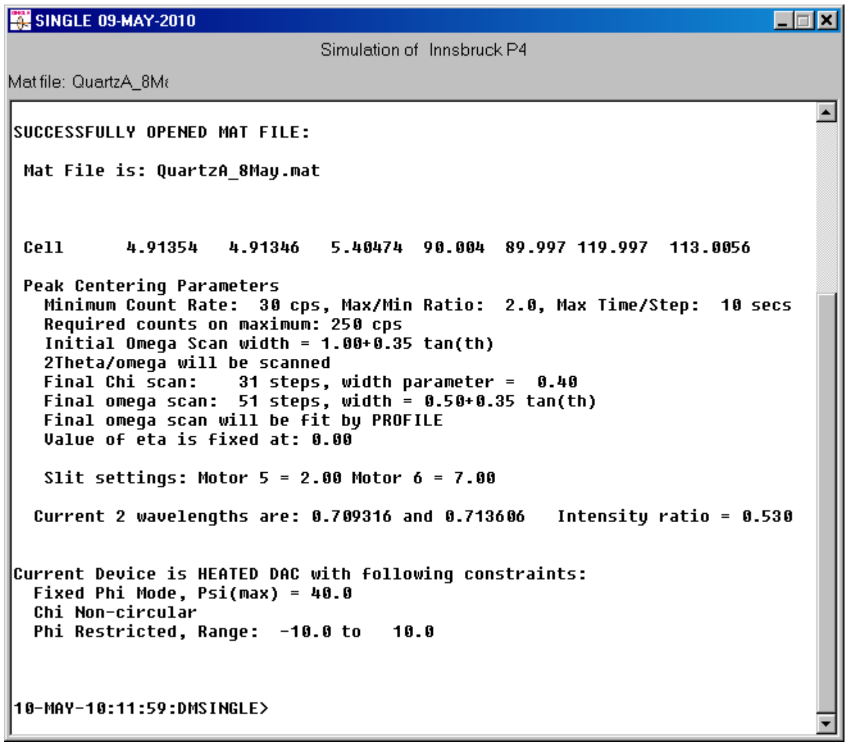
If the previous user did not exit the SINGLE software with the **exit** command, then the physical positions of the diffractometer will not necessarily be those of the **park** position, and an error message will have appeared. If this happens, check that the positions shown on the display match the physical positions of the diffractometer circles and slits. If not, correct with **ldmt**.

3.1. The SINGLE GUI

- You can type commands in to the terminal window by clicking anywhere in the window with the left mouse button, and then typing commands.
- Output from the SINGLE software also appears in this window, just like an "old-fashioned" terminal!
- There is no "type-ahead" buffer. You have to wait for the program to be ready to read your commands before typing them in. Be patient!
- When the diffractometer is busy, the terminal area will be grey, and no commands can be entered.
- On the upper part of the display there are two sections:
  - On the right side is information about the current diffractometer activity (the current action, shutter status, diffractometer angles and slit positions). The *hkl* values displayed here are calculated from the displayed angles with the current UB matrix.
  - On the bottom right are listed the names of the current mat and data files.
  - The behaviour of the counter display depends on the installation.
  - On the left side is a display of the last completed scan, with the angles and *hkl* at which it was performed. This is only updated at the end of the scan.

4. RUNNING THE PROGRAM WITHOUT THE DIFFRACTOMETER

SINGLE can also be used to perform diffractometer calculations without being connected to a diffractometer. To start in this “DMSINGLE” or “dummy” mode, select “Dummy” in the dialog box that appears when you start the program. After selecting the *mat* file the window should look something like this:



This version of the program will accept all commands except those that drive the diffractometer.

Even if you are using the code in *dummy* mode the SINGLE executable must be accompanied by a *difprof.dat* file for the machine for which you wish to do calculations.

5. COMMANDS

5.1. Diffractometer Control

Commands that control the diffractometer are only accessible if the computer is connected to a diffractometer. In DMSINGLE they are disabled.

cent - performs 1-position centering of the reflection currently in the detector window. If centering is successful the user is asked whether the resulting setting angles should be added to the reflection list.

cen8 - performs 8-position centering of the reflection currently in the detector window. If centering is successful the user is asked whether the resulting setting angles should be added to the reflection list. See information under **zref** for the definitions of offsets and zeroes.

clsh - closes the shutter.

cntr - performs 2-position centering (at +2θ and -2θ) of the reflection currently in the detector window. If centering is successful the user is asked whether the resulting setting angles should be added to the reflection list.

cone - performs cone search around a known reflection position. Diffractometer must be at the position of one reflection, and the 2θ and the angle to the second reflection is needed.

coun - performs a static count for 5 seconds at the current position.

cpos - reports current positions of the goniometer circles.

dcom - direct communication with the diffractometer controller. Only for use by experts for development, testing and configuration of the diffractometer controller.

demo - drives the diffractometer around a preset list of positions.

driv - drives the diffractometer to the last set of angles produced by CALC, if they were valid angles.

dvls - drives the diffractometer to the setting angles of a reflection in the list, if they are valid angles. User input: number of a reflection in the list.

filt - sets the filter wheel, if present.

fref - searches for reference marks on circles, if present. See local instructions before using. Not implemented for all types of diffractometer.

goto - inputs four angles and drives to that position.

half - sets half-slits on detector arm, if present.

halt - stops the diffractometer drives. See local instructions for exact action.

ldmt - redefines the current physical position of a motor to the value input by the user. User input: motor number, angle value.

WARNING: Read the Local Instructions for your diffractometer in the back of this manual before using this command. Also, take care not to enter an incorrect value as this may later cause physical collisions of the diffractometer. Take care redefining ω on diffractometers using absolute ω values - the safe method is to drive both 2θ and ω to values which you wish to define as zero.

mot - direct drive of individual motors. User input: motor number, target angle. The motors are numbered as follows: 1 = 2θ, 2 = ω, 3 = χ, 4 = ϕ. If diffracted-beam motorised slits are installed, those defining the opening in the ω-2θ plane are motor 6, the perpendicular set are motor 5. Motor 7 is the detector drive and motor 8 is the sample height.

opsh - opens the shutter. Consult local instructions as to action when the shutter is prevented from opening, for example by safety circuits.

park - drives the diffractometer circles to the park position.

phot – performs a rotation photograph scan.

prof - performs step scan of any diffractometer circle about the current position and outputs measured profile to the screen. The user is prompted for the motor number, step size, number of steps and count time per step.

ref - performs 2-position centering on reflections in the list whose use flags are set to 1. Updates the setting angles in the list for each successfully centred reflection. For failures the angles in the list are left unchanged, and the use flag set to 0.

srch - performs general search for reflection intensity, and lists positions of significant intensity to the screen. Does not do any centering.

step - performs step scan of any diffractometer circle with the shutter closed, without limit to the time the diffractometer waits at each step. Motion between the steps is done at slewing speed. The user is prompted for the motor number, the start and end points of the scan, the step size, and the time per step in minutes. The precision of the wait time at each step point is better than 2 seconds.

view - positions the diffractometer so that the sample can be viewed. See local instructions for exact action.

zero - drives all of the diffractometer circles to zero.

zref - performs 8-position centering on reflections in the list whose use flags are set to 1. Centering parameters can be reset with the SET CENT command. The slit settings on the detector are also defined by the parameters entered in SET CENT.

The user specifies whether the starting position for the centering process for each reflection is taken as the angles from the list, or is calculated from the indices in the list and the current UB matrix. For the purposes of instrument alignment it is possible to request zref to continue with a set of 8 equivalents after centering failures. This option should not be used for routine measurements.

The true angles of each reflection are determined from the eight equivalents by the method of King and Finger (*J. Appl. Cryst.*, 12, 374-378; 1979) and are put in to the reflection list. The reflection list intensity is the mean value of the intensity at each of the eight positions. For failures the angles in the list are left unchanged, and the use flag set to 0.

The crystal offsets reported by zref are defined on the Busing-Levy ϕ axis system (see above). The value of these offsets is the displacement of the crystal from the centre of the goniometer. Thus, to correct for a reported negative offset along the *y* axis, the crystal must be moved away from the X-ray source.

The circle zero errors reported by zref are the apparent values of the angles when the motor controller has set the angle to zero. Therefore to correct a circle zero errors:

- use **mot** to drive to the reported zero error.
- use **ldmt** to redefine this position as zero.

WARNING: Read the Local Instructions for your diffractometer in the back of this manual before using the **ldmt** command. Also, take care not to enter an incorrect value as this may later cause physical collisions of the diffractometer. Take care redefining ω on diffractometers using absolute ω values - the safe method is to drive both 2θ and ω to values which you wish to define as zero.

zrem - performs zref on multiple crystals, each of which must have a valid mat file, and all the mat must reside in the same folder.

5.2. Reflection List Manipulation and Crystallographic Operations

Crystallographic operations are performed upon the reflection list and upon the UB matrix (which also contains cell parameter information). The reflection list consists of up to 60 reflections. Each reflection entry consists of a list number, hkl, setting angles, the number of centred positions, a use flag, and the intensity. The list number is only the position of the reflection data in the list - some operations such as DEL or SORT lead to reallocation of list numbers to reflection data. The use flags are set with the USE command, and unset with the OMIT command.

Data entry into the reflection list may be made either by some of the commands INH, INA, or IND, or as the result of centering reflections on the diffractometer (CENT or CNTR).

Reflection indices may be input as command arguments as integers or reals. They are stored and manipulated by the program as reals, except when they are rounded to the nearest integer for calculations with COM, LSQ and CLSQ.

angl - calculates from the setting angles the angles between all reflections in the list with their use flags set to 1.

calc - calculates the setting angles of a reflection, hkl input by user. Three possible types of input:

- *hkl* only: the first equivalent position will be calculated (as in previous versions).
- *hkl a* : calculates all 8 equivalent positions of the reflection.
- *hkl n* : calculates the position of the *n*'th equivalent.

calp - calculates the 2θ and χ values of a reflection from the positions of spots measured on a rotation photograph. Input values are the distances between the spots on the photo.

cell - input of cell parameters by the user. Blank angle fields are set to 90^o.

clsq - performs symmetry-constrained refinement of the unit-cell parameters by the method of vector-least-squares by using the indices and setting angles of all reflections in the list with their use flags set to 1. The method used is that of Ralph and Finger (*J. Appl. Cryst.,* 15, 537-539; 1982). For trigonal unit-cells, the indexing is transformed to the hexagonal setting for the least-squares fit, and the results transformed back to trigonal.

com - calculates UB matrix from the unit cell parameters and two reflections in the list, selected by the user in terms of the list numbers. Before using this utility the user should have indexed the reflections with INDL. Note that COM rounds off the indices of reflections to the nearest integer.

del - deletes reflections from the list, as selected by list number. Sets of consecutive reflections may be selected by the end of the set being input as a negative number (see USE). List numbers of specific reflections left in the list are changed.

ina - inputs a set of setting angles into the list. Indices in the list are calculated from the current UB matrix.

ind - inputs a set of indices and setting angles into the list.

indc - performs an automatic indexing with all reflections in the list with their use flags set to 1. An alternative algorithm to AUTO.

indl - 3 sub-options: Clears all list indices to zero.
Inputs indices for individual reflections.
Indexes all reflections with the current UB matrix.

indx - indexes a set of setting angles input by the user according to the current UB matrix.

inh - inserts individual reflections into the list by inputting indices hkl. Setting angles in the list are calculated from the current UB matrix.

inl - inserts reflections by Laue group into the list by inputting indices hkl. Setting angles of all reflections under the Laue group (but not Friedel mates) are calculated from the current UB matrix, and those that are accessible, and not yet in the list, are added to the list.

list - outputs the reflection list to the terminal.

lsq - performs unconstrained least-squares determination of the UB matrix by using the indices and setting angles of all reflections in the list with their use flags set to 1. Outputs unit-cell parameters unconstrained by symmetry.

om - inputs UB matrix, with three values per line. Busing-Levy conventions. The unit-cell is calculated from the UB matrix.

omit - unsets the use flags of reflections in the list. The user inputs the list numbers. Sets of consecutive reflections may be selected by the end of the set being input as a negative number (see USE command).

pmat - lists the UB matrix, metric tensor, reciprocal metric tensor, U and B matrices on the terminal.

prom - lists the UB matrix on the terminal.

sort - sorts the reflection list. List numbers of specific reflections are changed. The sort can be made on 2θ, ω, χ, ϕ, h, k, l or intensity by entering 2,O,C,P,H,K,L or I respectively. To sort in descending order, precede the letter or number with a minus sign. Thus **sort** –C sorts the list by chi with the largest value first.

tlsq - performs symmetry-constrained refinement of the unit-cell parameters to *only the 2*θ angles of all reflections in the list with their use flags set to 1. This code written by Bob Downs.

tran - transforms the unit-cell parameters according to a 3x3 matrix input by the user. The UB matrix and the indices of all list reflections may also be transformed.

ubex – export the UB matrix to other diffractometer control systems. Conversion from the Busing-Levy UB matrix is performed with the transformation matrices loaded via the *difprof*.dat file.

ubim - import UB matrices from other diffractometer control systems. Conversion to the Busing-Levy UB matrix is performed with the transformation matrices loaded via the *difprof*.dat file, and the unit-cell is calculated.

use - sets the use flags of reflections in the list. The user inputs the list numbers. Sets of consecutive reflections may be selected by the end of the set being input as a negative number. Thus 4,-7 would indicate reflections 4,5,6, and 7. Reflections with numbers not input have their use flags unchanged upon exit.

5.3. Data Collection

Data collection parameters such as scan type, width, step size, 2θ limits etc are chosen with **set data**. This information is displayed on the terminal when any of these commands is input, and before the data collection starts. Data is stored as step scans in an ASCII file selected with the **set datfile** utility.

dc s - initiates a data collection scan over a set of reflections. Indices are generated by the program subject to the limits provided by the user in SET DATA.

dc l - initiates a data collection scan over a list of reflections. The list may be either an ASCII file with one set of hkl per line, or the reflections in the reflection list whose use flags are set to 1.

dc i - initiates a data collection scan over single reflections. The user is prompted for the hkl of each reflection in turn.

dc p - performs a psi scan of a single reflection.

scan - performs a linear scan in reciprocal space.

5.4. General Utilities

The utility commands include:
- **exit** to park the diffractometer and exit from the SINGLE program.
- **help** to see a list of commands.
- **macr** to load a text file of commands and run them.
- **note** to make notes into the log file.

- **set** to set many parameters including the diffraction geometry and device restrictions (e.g. DAC mode, or furnaces), centering, data scan parameters etc. and to set additional logging options for debugging problems.
- **show** to display parameters.
- **test** for testing of software developments. Do not use.

6. COMMAND LIST SUMMARY

In this list the "arguments" column details the arguments that can be entered on the same line as the command itself. If no argument is given the program will provide a prompt for the required input.

Many commands will also issue questions for the user to answer.

Command	Description	Arguments
ANGL	Calculates from the setting angles the angles between all reflections in the list with their use flags set to 1.	none
CALC	Calculates the setting angles of a reflection	h,k,l,n or A
CALP	Calculated the 2θ and χ angles of a reflection from the coordinates of spots on a rotation photograph	Δx,Δz
CELL	Inputs of cell parameters by the user. Blank angle fields are set to 90^o.	a,b,c,α,β,γ
CENT	Performs 1-position centering of the reflection currently in the detector window.	None
CEN8	Performs 8-position centering of the reflection currently in the detector window.	None
CLSH	Closes the shutter	None
CLSQ	Performs symmetry-constrained refinement of the unit-cell parameters by the method of vector-least-squares by using the indices and setting angles of all reflections in the list with their use flags set to 1.	crystal-system number (1-7)
CNTR	Performs 2-position centering (at $+2\theta$ and -2θ) of the reflection currently in the detector window.	None
COM	Calculates UB matrix from the unit cell parameters and two reflections in the list	two list numbers
CONE	Performs a cone search	None
COUN	Performs a static count for 5 seconds at the current position.	None
CPOS	Reads motor positions from motor controller	None
DC I	Initiates a data collection scan over single reflections. The user is prompted for the hkl of each reflection in turn	None
DC L	Initiates a data collection scan over a list of reflections. The list may be either an ASCII file with one set of hkl per line, or the reflections in the reflection list whose use flags are set to 1.	None
DC P	Performs a psi scan of up to 30 reflections.	none
DC S	Initiates a data collection scan over a set of reflections. Indices are generated by the program subject to the limits provided by the user in **set data**	None
DCOM	Direct control of the interface. For experts only!	None
DEL	Deletes reflections from the list, as selected by list number. Sets of consecutive reflections may be selected by the end of the set being input as a negative number. List numbers of specific reflections left in the list are changed.	list numbers
DEMO	Drives the diffractometer around a preset list of positions.	None
DRIV	Drives the diffractometer to the last set of angles produced by CALC, if they were valid angles	None
DVLS	Drives the diffractometer to the setting angles of a reflection in the list, if they are valid angles.	list number
EXIT	Parks the diffractometer and exits from the program	None
FILT	Sets the filter wheel, if present.	filter number
FREF	Starts the diffractometer controller searching for the reference marks on each of the circles.	None
GOTO	Drives to requested angles	2θ, ω, χ, ϕ

HALF	Sets the half-slits if present	T=top, B=bottom, L=left, R=right O=open
HALT	Stops the diffractometer drives	None
HELP	Provides a list of commands	None
INA	Inputs a set of setting angles into the list. Indices in the list are calculated from the current UB matrix.	None
IND	Inputs a set of indices and setting angles into the list.	None
INDC	Performs an automatic indexing with all reflections in the list with their use flags set to 1.	None
INDL	3 sub-options: Clears all list indices to zero. Inputs indices for individual reflections. Indexes all reflections with the current UB matrix.	None
INDX	Indexes a set of setting angles input by the user according to the current UB matrix	setting angles
INH	Inserts reflections into the list by inputting indices hkl. Setting angles in the list are calculated from the current UB matrix.	None
INL	Inserts reflections in to the list by Laue group	Laue group
LDMT	Redefines the current physical position of a motor to the value input by the user.	motor number, angle
LIST	Outputs the reflection list to the terminal.	None
LSQ	Performs unconstrained least-squares determination of the UB matrix by using the indices and setting angles of all reflections in the list with their use flags set to 1. Outputs unit-cell parameters unconstrained by symmetry.	None
MACR	Loads a text file of commands and runs them.	None
MOT	Direct drive of individual motors.	motor number, angle
NOTE	Allows text to be typed on the terminal to be echoed to the user logfile, without being interpreted as commands. Exit from the utility by typing EXIT on a line on its own.	None
OM	Inputs UB matrix, with three values per line.	None
OMIT	Unsets the use flags of reflections in the list. The user inputs the list numbers. Sets of consecutive reflections may be selected by the end of the set being input as a negative number. Thus 4,-7 would indicate reflections 4,5,6, and 7. Reflections with numbers not input have their use flags unchanged upon exit	list numbers
OPSH	Opens the shutter	None
PARK	Drives the diffractometer to the preset park positions	None
PHOT	Performed rotation photo scan, starting from preset *photo* position	None
PMAT	Prints current G, G*, U and B matrices	none
PROF	Performs step scan of any diffractometer circle about the current position and outputs measured profile to the screen	none
PROM	Prints the current UB	none
REF	Performs 2-position centering on reflections in the list whose use flags are set to 1. Updates the setting angles in the list for each successfully centred reflection. For failures the angles in the list are left unchanged, and the use flag set to 0.	none
SET CENTER	Inputs parameters for centering reflections	none
SET DATA	Inputs data collection parameters	none
SET DATFILE	Opens a file for storing scans from data collection	none
SET DEVICE	Selects diffraction geometry and restrictions due to devices (e.g. DAC)	none

SET LOG	Sets logging options	none
SET MATFILE	Selects mat file	none
SET TITLE	Inputs a title	none
SET WAVE	Inputs wavelengths	
SCAN	Performs a linear scan in reciprocal space	none
SHOW CENTER	Lists parameters for centering reflections	none
SHOW DATA	Lists data collection parameters	none
SHOW DATFILE	Prints name of the file for storing scans from data collection	none
SHOW DEVICE	Shows the selected diffraction geometry and restrictions	none
SHOW DEVTYPES	Lists all available device types	none
SHOW LOG	Shows logging options	none
SHOW MATFILE	Prints the name of the mat file	none
SHOW TITLE	Prints the title	none
SHOW UB	Prints the UB matrix	none
SORT	Sorts the reflection list. List numbers of specific reflections are changed.	+ or -, followed by 2,O,C,P,H,K,L, or I
SRCH	Searches for reflections	none
STEP	Performs step scan of any diffractometer circle with the shutter closed	none
TEST	Command to allow testing of software developments. Do not use!	none
TLSQ	Performs symmetry-constrained refinement of the unit-cell parameters to *only the* 2θ angles of all reflections in the list with their use flags set to 1.	crystal-system number (1-6)
TRAN	Transforms the unit-cell parameters according to a 3x3 matrix input by the user. The UB matrix and the indices of all list reflections may also be transformed.	none
UBEX	Exports UB matrix to other diffractometer control systems.	None
UBIM	Imports UB matrix from other diffractometer control systems	None
USE	Sets the use flags of reflections in the list. The user inputs the list numbers. Sets of consecutive reflections may be selected by the end of the set being input as a negative number. Thus 4,-7 would indicate reflections 4,5,6, and 7. Reflections with numbers not input have their use flags unchanged upon exit	list numbers
VIEW	Drives diffractometer so that the sample can be viewed with the telescope	none
ZERO	Drives the diffractometer circles to zero	none
ZREF	Performs 8-position centering on reflections in the list whose use flags are set to 1. Updates the setting angles in the list for each successfully centred reflection. For failures the angles in the list are left unchanged, and the use flag set to 0.	none
ZREM	Does ZREF on multiple crystals	none

The following commands available in earlier versions have been discontinued:

Command	Description
AUTO	Performed an automatic indexing with all reflections in the list with their use flags set to 1. The resulting unit-cell is normally reduced. The reflections are indexed.
BRAV	Cell reduction routine
CALI	Calibration routine
FACE	Orientation of crystal faces with respect to the telescope
GRID	Performed static intensity measurements at points of a grid defined in reciprocal space
LOG	Replaced with SET LOG
OMX	Replaced with UBIM
POW	Performed a powder diffraction scan (i.e. 2θ) and recorded profile in an ascii file.
PRNT	Turned printer on and off.

7. ERRORS

Errors in the program or the diffractometer are of two levels:

WARNING: Non-fatal error which the software will either ignore or attempt recovery. Examples are:

- individual failures in communications,
- individual failure to open shutter,
- failure to open files,
- software failures (unusual results, failure of least-squares),
- failure of user to specify necessary information,
- problems reading the mat file.

The program will log the warning to the user log, the terminal, and the instrument log. If communication or instrument problems continue, a fatal error will be logged. If they are cleared, then the program will issue a message noting the recovery, that again will be logged to the user log, the terminal, and the instrument log.

FATAL ERROR: Examples are:

- failures in reading the *difprof.dat* file,
- diffractometer limit switches active,
- shutter failure after 5 attempts,
- persistent error in communications.

These force the program to stop, request acknowledgement from the operator, and return the program to the main prompt to allow appropriate action to be taken by the operator. Fatal errors are logged to the user log, the terminal, and the instrument log.

Persistent fatal errors should be investigated before they lead to damage to the diffractometer!

STOP BUTTON: The exact operation of the stop button depends on the type of motor controller. For details see local operation notes below. In general, on Huber SMC controllers, the STOP button always stops motions immediately. On other interfaces, it stops the program and the diffractometer at the end of the current drive or scan.

Use of the button forces the program to stop, request acknowledgement from the operator, and return the program to the main prompt. Use of the STOP button is logged to the user log, the terminal, and the instrument log.

8. GENERAL EXPERIMENT INSTRUCTIONS

These instructions are only intended as a general guide to the sequence of operations required to obtain unit-cell parameters from a crystal mounted in a pressure cell. SINGLE commands are shown in **bold**.

1. Start:
    a. If this is a new pressure point for a crystal that has previously been measured, make a copy of the previous mat file and rename it.
    b. Start SINGLE.
    c. For a new pressure point on a crystal, select the new mat file. For a completely new crystal, create a new matfile by typing in a new name in the file browser.

2. Mounting the cell:
    a. Mount the goniometer head with the DAC on to the goniometer.
    b. If necessary, drive the diffractometer to zero: **zero**.
    c. Check that the DAC is perpendicular to the beam. Adjust if necessary.
    d. Drive the diffractometer to the view position: **view**.
    e. Optically center the gasket hole.
    f. Exit from the view utility. Remove the telescope if necessary.

3. Determining an approximate UB for a new crystal:
    a. Set the software to DAC mode: **set dev**.
    b. If you have a UB matrix from an Oxford Diffraction CCD instrument, input the UB matrix from Crysalis: **omx**.
    c. If you have a UB matrix from another type of instrument, transform the UB matrix to the Busing-Levy axial system, and input the resulting matrix to SINGLE: **om**.
    d. If you do not have a UB matrix, you can either make a manual search (**opsh, mot**) or a search with SINGLE: **srch**. Center any reflection that is found: **cntr**. Index it in the list: **indl**.
    e. Once you have found one reflection, and you know the unit-cell parameters, you can also use the cone search: **cone**.
    f. Continue until you have two centered and indexed reflections.
    g. Go to section 5.

4. Determining an approximate UB for a crystal measured at a previous pressure:
    a. Calculate the position of a strong reflection: **calc**.
    b. Drive the diffractometer to this position: **driv**.
    c. Open the shutter: **opsh**.
    d. If there is no reflection in the detector, search first on ω: **mot 2,*.** Most sample crystals do not move more than 1 or 2 degrees on ω between pressure points.
    e. If you do not find the reflection within $\pm 5^{o}$, open up the vertical detector slit (**mot 5,*** if motorized, manual adjustment if not) and repeat the search in ω (**mot 2,***). If you still do not find it, change χ by 5^{o} and search in ω again.
    f. When you have found the reflection, scan it in ω: **prof**.
    g. Drive to the maximum in ω: **mot 2,***.
    h. Make sure that the vertical slit is set to the correct width for centering.
    i. Center the reflection in 2 positions: **cntr**. When complete add the reflection to the list.
    j. Do the same for a second reflection.

5. Determining an approximate UB:
    a. Reindex the two reflections with integer indices: **indl**.
    b. Input your best guess for the new cell parameters (e.g. by extrapolation to this new pressure): **cell**.
    c. Calculate the new UB matrix from the two reflections: **com**.
    d. If the calculated and measured angles between the reflections differ by a large amount, it is likely the indexing or unit-cell parameters are wrong. Sort it out by trying to re-index one of the reflections.
    e. If the calculated and measured angles between the reflections differ by 0.3 – 5^o, it is likely the indexing is correct, but your unit-cell parameters are wrong. Or, you may have reflections from two different crystals, or your sample crystal may be moving.
    f. If the calculated and measured angles between the reflections differ by less than 0.3^o, then you probably have a valid UB. Check that other reflections can be found with the approximate UB: **calc**, **driv**, **prof**. If not, go back and fix the problem.

6. Correcting offsets (This is normally only necessary for a new crystal, or if the goniometer head has been adjusted).
    a. Insert the indices of one strong reflection in to the list with **inh** (or use one of the centered reflections).
    b. Clear all "use flags" for all other reflections in the list: **omit**.
    c. Center the reflection in 8 positions: **zref**.
    d. At the end of zref, correct the crystal position.
    e. Repeat this procedure until the offsets are small (typically <0.05mm).
    f. Note: An alternative to using a list reflection is to drive to a reflection and use the **cen8** command to perform the 8-position centering.

7. Measuring the unit-cell parameters:
    a. For a new crystal, input a list of reflections to be centered with **inl** (by Laue group) or individually with **inh**.
    b. For a measurement of an old crystal, review the list of reflections with **list**. Make sure the reflections you want centered have the use flag set to 1. Commands **use** and **omit** change the value of the use flags.
    c. Start 8-position centering; **zref**.
    d. At the end, determine the cell parameters unconstrained by symmetry; **lsq**.
    e. Determine the cell parameters constrained by symmetry; **clsq**.

8. For expert users only:
    a. You can set up the different mat files for two (or more!) crystals in a DAC, and then start 8-position centering on all of them with **zrem**.

9. LOCAL INSTRUCTIONS

BAYREUTH "OLD HUBER" OPERATION NOTES

This is the diffractometer in the Xray lab in Bauteil 2. It is run on an SMC9000 controller.

1. Motor drives are in degrees, slits in mm. For centering the usual slit sizes are motor5 = 1mm, motor6 = 9mm.
2. The SMC9000 motor numbers normally correspond to the assignment of motor numbers in SINGLE, but are always taken from the *difprof.dat* file.
3. The program works with ω values as the deviation from bisecting. The ω values displayed by the SMC9000 are absolute ω: $\omega(\text{abs}) = \omega(\text{bi}) + \theta$.
4. Because of limitations of the SMC9000 interface, the count times of stationary counts (e.g. from the command **coun**) are rounded to the nearest second.
5. The counter display on the GUI is not updated during scans. After a scan is plotted, the counter display shows the maximum count rate in the scan.
6. WARNING: Take care redefining ω with **ldmt.** The safe method is to drive both 2θ and ω to physical zero, and then use **ldmt** to set 1,0 and 2,0 *in this order*.
7. The stop button is inactive except when the diffractometer is moving. Pressing the button when the diffractometer is stationary will have no effect. The stop button halts motor drives and scans immediately.
8. After stopping the SINGLE program during a measurement, carefully check that the SMC9000 controller and the software display the same motor positions (allowing for the difference between bisecting ω displayed by the program and absolute ω displayed by the controller (see (3) above).
9. If a motor limit switch is activated by the diffractometer, the SINGLE program will detect the limit switch and halt with an error message. When you select "OK" the program will return to the SINGLE prompt. Once a limit switch is detected by the SMC9000 it will not accept any further commands from the computer. It is therefore *critical* that you now complete the following instructions:
    a. Clear the error flag from the SMC9000 controller by pushing the "RESET" button. If the "limit switch" message reappears on the SMC9000 then the limit switch is still active and you will have to move the diffractometer manually to clear the switch, and then RESET again.
    b. Read the physical positions of the diffractometer circles and the slits from the odometers.
    c. The RESET clears the motor positions from the SMC9000 controller. Use the **ldmt** command to reload the correct physical positions of the circles and slits into the SMC9000. Remember to allow for the fact that the SMC9000 displays ω as absolute, whereas SINGLE uses ω relative to bisecting.
    d. When you have loaded all six motor positions with **ldmt** drive each circle to zero with the **mot** command. Watch the diffractometer carefully because if you made an error in step *b* or *c* you will have a collision. Check the odometer. If the motor is not at physical zero, reset the position with **ldmt.** Continue until the motor is at physical zero, and the position displayed by both the SMC9000 and SINGLE is zero. Do the axes in this order: ϕ, then χ, then 2θ, then ω.
    e. When all circles are zeroed, check the motion of the slits by driving them to other non-zero values. Do not drive the slits to zero!
    f. If all appears ok, try **calc** and **driv** to a known reflection position.
10. The "counts" display on the GUI normally shows the maximum from the last scan that was performed unless the **coun** command is used, in which case the measured count rate is displayed.

BAYREUTH “NEW HUBER” OPERATION NOTES

This is the diffractometer combined with the Brillouin spectrometer in Bauteil 6. It is run on an SMC9300 controller. Operations are the same as the VTX Huber except:

1. Motors 1,2,3,4 are 2θ, ω, χ and ϕ respectively.
2. Motor 5 on the controller is the sample height drive, designated as motor 8 within SINGLE.
3. Circles χ and ϕ are set non-circular to prevent damage to cables.
4. There are no motorised diffracted beam slits, but the size of the diffracted beam slits must be loaded in to SINGLE with the **ldmt** command.

VTX HUBER OPERATION NOTES (SMC9300 Controller)

1. Motor drives are in degrees, slits in mm. For centering the usual slit sizes are motor5 = 2mm, motor6 = 9mm.
2. The SMC9300 motor numbers normally correspond to the assignment of motor numbers in SINGLE, but are always taken from the *difprof.dat* file.
3. The program works with ω values as the deviation from bisecting. The motor controller uses absolute ω: ω(abs)= ω(bi)+θ.
4. The counter display on the GUI is not updated during scans. After a scan is plotted, the counter display shows the maximum count rate in the scan.
5. WARNING: Take care redefining ω with **ldmt.** The safe method is to drive both 2θ and ω to physical zero, and then use **ldmt** to set 1,0 and 2,0 *in this order*.
6. The stop button is inactive except when the diffractometer is moving. Pressing the button when the diffractometer is stationary will have no effect. The stop button halts motor drives and scans immediately.
7. After stopping the SINGLE program during a measurement, carefully check that the software displays the physically motor positions by comparing the displayed values to the physical positions of the goniometer (allowing for the difference between bisecting ω displayed by the program and absolute ω displayed by the controller (see (3) above). Normally the displayed positions will be correct.
8. If a motor limit switch is activated by the diffractometer, the SINGLE program will detect the limit switch and halt with an error message. When you select "OK" the program will return to the SINGLE prompt. Then:
    a. Read the physical positions of the diffractometer circles and the slits from the odometers and compare them to the values displayed on the SINGLE GUI. Write them down.
    b. Use the SMC9300 controller to move the diffractometer off the limit switch.
    c. In SINGLE, reinitialise the motor controllers with **ldmt**.
    d. Drive the motors to zero and recheck the odometer values.
    e. When all circles are zeroed, check the motion of the slits by driving them to other non-zero values. Do not drive the slits to zero!
    f. Close and re-open the program.
    g. If all appears ok, try **calc** and **driv** to a known reflection position.
9. The "counts" display on the GUI normally shows the maximum from the last scan that was performed unless the **coun** command is used, in which case the measured count rate is displayed.

STADI4 OPERATION NOTES

1. Motor drives are in degrees, slits in mm. The slits can only be adjusted manually. Use **ldmt** to enter the values of the slit sizes in to SINGLE. The slit closer to the crystal is the vertical aperture (motor 5) and the slit closer to the detector sets the horizontal aperture (motor 6) For centering the usual slit sizes are motor5 = 2mm, motor6 = 7mm.
2. The program works with ω values as the deviation from bisecting. The ω values used and displayed by the Stoe motor controller are absolute ω: $\omega(abs)= \omega(bi)+\theta$.
3. The Stadi4 motor controller is set by SINGLE to be non-circular for χ and ϕ at all times.
4. If you move the diffractometer with the manual control box, you must update the circle positions in SINGLE with the **cpos** command.
5. The counter display on the GUI is not updated during scans. After a scan is plotted, the counter display shows the maximum count rate in the scan.
6. WARNING: Take care redefining ω with **ldmt** because of (2). The safe method is to drive both 2θ and ω to physical zero, and then use **ldmt** to set 1,0 and 2,0 *in this order.*
7. The stop button is inactive except when the diffractometer is moving. Pressing the button when the diffractometer is stationary will have no effect. Due to a limitation of the Stoe motor controller, the stop button will not halt motor drives immediately, but will allow the current drive to be completed before the program is stopped. During scans, pressing the stop button stops the diffractometer at the end of the scan.
   a. After stopping the SINGLE program during a measurement, carefully check that the Stoe motor controller and the software display the same motor positions (allowing for the difference between bisecting ω displayed by the program and absolute ω displayed by the controller (see (2) above).
8. If a motor limit switch is activated by the diffractometer, the SINGLE program will detect the limit switch and halt with an error message. When you select “OK” the program will return to the SINGLE prompt. Once a limit switch is detected by the Stoe motor controller it will not accept any further commands from the computer. It is therefore *critical* that you now complete the following instructions:
   a. Clear the error flag from the Stoe motor controller by driving the circles manually until the limit switch is no longer active.
   b. Issue the **cpos** command in SINGLE to read the circle positions from the Stoe motor controller. If you get error or warning messages (quite normal), repeat the command until it executes without warnings or errors. If this does not happen, exit and restart SINGLE.
   c. Now *very carefully* check that the positions displayed in SINGLE and the positions displayed by the Stoe motor controller are identical (allowing for the difference between bisecting ω displayed by the program and absolute ω displayed by the controller (see (2) above).
   d. Check that all is ok by performing the search for reference marks **fref** (see 10 below).
   e. If all appears ok, try **calc** and **driv** to a known reflection position.
9. The use of the reference positions: **fref.** This command tells the Stadi4 controller to spin the circles until the reference switch is activated. The drives are always made in a negative direction from the current position, so all of the diffractometer circles must be at a positive position.
   a. First use **mot** or **goto** to drive the diffractometer to positive positions. Usually **goto 2,2,2,5** will be ok. If the positions have been lost, then make sure the diffractometer is physically set at positive positions. The actual values of the angles in the controller do not matter.
   b. Issue the **fref** command. The diffractometer drives each circle in turn to the reference position. If the diffractometer starts at a negative position, then it will drive to a limit switch. If this happens, recover from the problem (see section 10 above) and start the procedure again, *but this time make sure that the diffractometer is at positive positions!*

c. After **fref** procedure is complete, the diffractometer is at the physical reference marks. You must now check that the values of the diffractometer circle positions in the controller and on the Single GUI are correct, by comparing with the values recorded in the log book of the instrument. Do not forget that with the Stadi4 controller displays absolute omega, while the GUI displays relative omega (see 2). If necessary, use **ldmt** to reinitialise the motor positions.
d. Now check the zeroes are correct by **calc** and **driv** to a reflection.

10. If you have a video microscope system:
    a. Type **view** to drive the diffractometer to the viewing system.
    b. Put on the video microscope, and attach its power cable.
    c. Click on the icon on the desktop: *shortcut to MicroVid4L*. When a dialog box appears saying the program cannot drive the ϕ axis, click ok. A window with the picture from the camera will appear.
    d. The scale on the video display is wrong. Each division is approximately 20 micron (0.020mm).
    e. Center the crystal using the positions available in the **view** utility. Do not use the manual control box. If you do, you must follow the instructions in (5) above.
    f. On completion of centering:
        i. Close the video display software.
        ii. Unplug the power cable, remove the camera from the diffractometer.
        iii. Exit from the **view** utility.
11. If the power goes off, then the diffractometer interface may need to be reinitialised.
    a. If the diffractometer was sitting at zero, no reinitialisation should be necessary.
    b. Otherwise, reinitialise the positions with **ldmt**. Then find the reference positions, following the instructions in 10 above.

P4 OPERATION NOTES

1. The slits can only be adjusted manually. Use **ldmt** to enter the values of the slit sizes in to SINGLE. For centering the usual slit sizes are motor5 = 2mm, motor6 = 7mm. On the diffractometer, the front slit (i.e. nearest the crystal) is the horizontal slit (motor 6) and is always left fully open, with the slot in the adjustment screw horizontal. The back slit is the vertical aperture (motor 5) and is usually set with the slot in the adjustment screw at 45^{o}.
2. The SINGLE program works with ω values as the deviation from bisecting. The ω scale on the diffractometer reads absolute ω values: $\omega(abs)= \omega(bi)+\theta$.
3. The P4 motor controller is set by SINGLE to be non-circular for χ and ϕ at all times, from the entries in the *difprof*.dat file.
4. If you move the diffractometer with the manual control box, you must update the circle positions in SINGLE with the **cpos** command.
5. Count times shorter than 0.25 seconds are not permitted, as they seem to cause a communication problem with the diffractometer controller. Requests for count times less than 0.25 seconds are changed to 0.25
6. The counter display is updated with the latest step count during scans. At the end of the scan, the display is set to the maximum count rate found in the scan.
7. If **ldmt** is used to reset circle positions (not the slits), you **must exit** and restart the program before continuing.
8. The stop button on the SINGLE GUI is inactive except when the diffractometer is moving. Pressing the button when the diffractometer is stationary will have no effect. Due to a limitation of the P4 motor controller, the stop button will not halt motor drives immediately, but will allow the current drive to be completed before the program is stopped. During centering, pressing the stop button stops the diffractometer at the current point in the scan.
9. After power glitches, or switching between Xscans and Single, it is possible for the communications buffer of the Siemens P4 motor controller to get de-synchronised. In Single this will result in unusual operations or drive error messages.
    a. The test to determine if you have this problem is in SINGLE to drive the diffractometer to non-zero 2θ and then issue a **coun** command. If the screen becomes white again immediately you have the comm problem. If the screen goes grey for 5 seconds, you do not have the problem.
    b. A second test can be done in Xscans. Do a drive of motors. If the program does not return automatically to the drive menu after the motors stop, you have this comm problem.
    c. The solution is to exit all control programs and reset the P4 controller with the red reset button on the front of the controller. Wait until the reset and reload of the firmware is complete (as indicated by the diffractometer motions stop and the red light on the floppy drive in the controller is off). Then restart SINGLE. Repeat the test as in (a).
10. If the Siemens P4 controller is powered off and on again, the motors may be moved by the controller, but the controller may still report their positions as zero. Therefore after powering up the controller, check the positions of all circles as indicated by the scales on the instrument. Correct with **ldmt** if necessary.
11. If a motor limit switch is activated by the diffractometer, the SINGLE program will detect the limit switch and halt with an error message. When you select "OK" the program will return to the SINGLE prompt. You ***must*** follow these instructions:
    a. Hold down "Limit override" button on P4 controller.
    b. Use **mot** to drive the circle off the limit (carefully!!).
    c. Release "Limit override" button.
    d. Drive all circles carefully to zero and check zeroes on scales on diffractometer.

e. Do a **zref** on a reflection to check zeroes.

ADDITIONAL BOULDER P4 OPERATION NOTES

1. Read the general P4 operation notes as well!
2. The shutter is not controlled by the Siemens controller, so there is no control of the shutter from SINGLE, nor is there any feedback of the shutter status from the controller. The shutter must be opened and shut manually from the generator controller.