

SINGLE - 04
DISTRIBUTION NOTES
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1. Follow the instructions in this section **only**. The information under the heading “07-February-05” is provided for background information on earlier upgrades.
2. To install this version as an upgrade, follow the instructions in section 2 of the Installation guide. Do not copy the *difprof.dat* file if this is an upgrade. To make a completely new installation follow the instructions in section 1 of the Installation guide.
3. This version contains minor bug fixes and internal code changes from the version of 7-February 2005:
 - a. Further modified code for VT configuration to better interlock shutter with doors on radiation enclosure.
 - b. Restructured code for driving detector slits. No user-visible changes on diffractometers with motor-driven slits. On machines without motor-driven slits the variable DSLIT in the **CONFIG** line of *difprof.dat* should be set to 0. Then the default widths (in mm) of the slits are loaded on program startup from the “park” position listed in *difprof.dat*. The program can then be told about changes in the slit widths with *ldmt* command, using motor numbers 5 and 6.
 - c. Fixed bug in reading of mat file that corrupted *hkl* indices < -9 or >9
 - d. Fixed bug in **del** command that stopped groups of reflections being deleted from the command line.
 - e. Added extra motor position checking and error reporting in the AMS version.

07-February-05

1. To install this version as an upgrade, follow the instructions in section 2 of the Installation guide. The installation guide and manual contain revisions and should be copied. Do not copy the *difprof.dat* file if this is an upgrade. Instead you will edit your existing version of this file (see below).
2. New features compared to versions of summer 2004:
 - a. Changes to SMC9000 communications to handle longer instruction strings.
 - b. **GOTO** command allows you to drive to a set of angles.
 - c. Prevent user from using **set device** to set circles circular when the *difprof.dat* file has the default configuration as non-circular.
 - d. Changed screen buffer handling to try to prevent screen “freezing up”
 - e. Add warning to end of **view** command.

- f. Fixed various little bugs.
 - g. Changed handling of motor step errors in AMS version.
 - h. Introduced optional checking of shutter status (see below)
3. Checking the shutter status.
- a. Some diffractometer systems provide feedback from the shutter controller to the computer and the SINGLE program on whether the shutter is open or not. When this is provided that program always makes sure that the shutter status (open/shut) is the same as the program requested. If it is not, then the program logs an error and stops.
 - b. This functionality used to be “hard-wired” in to the code. In order to make distribution easier, optional shutter status checking has been introduced. If your hardware returns a shutter status to the computer (e.g. Bayreuth and Heidelberg Huber systems) then the last digit of the CONFIG line in *difprof.dat* should be a 1:
CONFIG -1,-1,-1,-1,0,0,0,1,0,0,500,1
 - c. If you do not have feedback, or wish to disable it for testing, change this last digit to a zero: **CONFIG** -1,-1,-1,-1,0,0,0,1,0,0,500,0

4. Notes on the zref slit settings.

- a. The use of preset values was introduced in order to allow a change in the future to have each mat file contain information on more than one crystal.
- b. When you start **zref** the slits will be driven to the preset values. These values are stored in the matfile of your sample crystal. You can change these preset values for the current crystal with the **set centre** command.
- c. The default values these slit settings for your instrument are also stored in the *difprof.dat* file. These values are used when you create a new matfile on startup of Single (see section on Files in the Single manual).
- d. You should edit the *difprof.dat* file to include the default slits settings for zref. On the SCANS1 line add at the end the default settings for motors 5 and 6. For example, for default settings of motor 5 = 2.0mm and motor 6 =9.0 mm, change the line in the *difprof.dat* file from:

SCANS1 30.0,2.0,10.,250.,1.0,0.35

To

SCANS1 30.0,2.0,10.,250.,1.0,0.35,2.0,9.0

MINCT,MAXMIN,TMAX,maxct,OMW_I1,OMW_I2,M5default,M6default