

SINGLE2010

Distribution Notes

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This is just a list of the more important changes made to the code, what changes you need to make to your instrument configuration and *difprof.dat*, and what changes you can expect in the results. Full information is given in the *Installation Guide* and the *Users Manual*.

1. The Huber SMC9300 motor controllers are normally configured and shipped by Huber so that they report 3 decimal places for each motor position to Single. This was not documented by Huber. This meant that if your diffractometer worked with motor steps that were not an exact multiple of 0.001deg (e.g. 400 steps/deg is 0.0025deg/step) then the controller reported positions incorrect by 0.0005deg. If you have a Huber diffractometer with one of these controllers, read the section on SMC9300 controllers in the *Installation Guide* to reconfigure the controller correctly. Making this change will reduce the *esd*'s on your measured unit-cell parameters!
2. The monochromator code has been corrected and tested and shown to be correct. If your instrument has a monochromator, you will get slightly different unit-cell parameters with smaller *esd*'s than with previous versions.
3. The handling of furnaces is much improved. Further developments will be made over the next year if needed.
4. There are lots of new commands – see the Version Notes in either the *Installation Guide* or the *Users Manual* for changes and new commands, and the *Users Manual* for details of the commands. In particular:
 - a. The data collection commands have been renamed
 - b. CALC now can report 8 positions, or any one of 8 equivalents
 - c. OMX has been replaced by a more general import/export utility for orientation matrices. Read the information in Section 5 of the *Installation Guide* on UBTRAN to configure this facility.
 - d. There is a macro utility.