Cal_Par

I. Description

This program use the output file of PSM3 (output_name.hkl or output_namefin.hkl) to evaluate cell parameters (except for triclinic or rhmbohedral cell) by linear least square refinement on the g^2 values.

II. Use

Put the output file of PSM3 and Cal_Par.exe in the same directory and double click on Cal_Par.exe.
Enter the name of the output file of PSM3
Ex : testfin.hkl
Number of reflections in the file are displayed
The cell symmetry is asked. Type the letter corresponding to the symmetry of your compound.
Ex : o
The program calculates the cell parameters from different parts of the reciprocal space considering the g values. You have then to put a g_{min} and a g_{max} value.
It do similar cuts with intensity. You have to enter a I/σ maximum, typically 5 or 6.
Cell parameters are displayed for many parameters and the final values are display at the end together with deviation. Chi2 is calculated and display as well as chi2/number_of_reflexions (this value should be below 0.000020).

NB : Displayed cell parameters quality depend of the quality of the calibration.