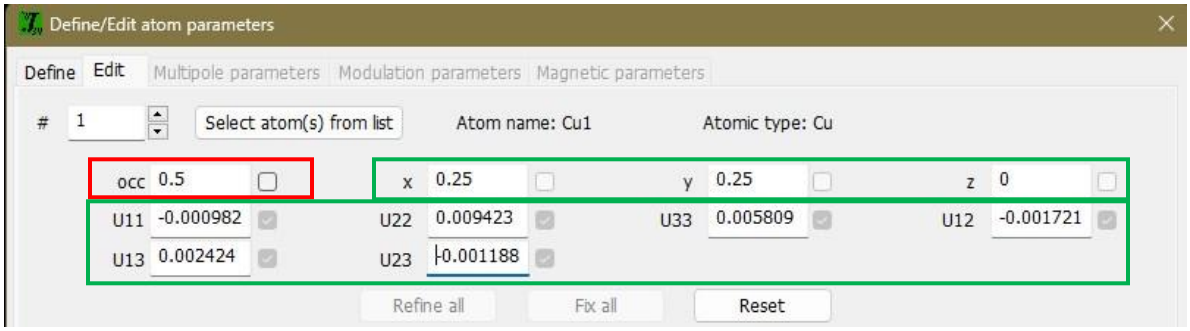
This is taken from our paper: DOI 10.1515/zkri-2014-1737 Z. Kristallogr. 2014; 229(5): 345–352

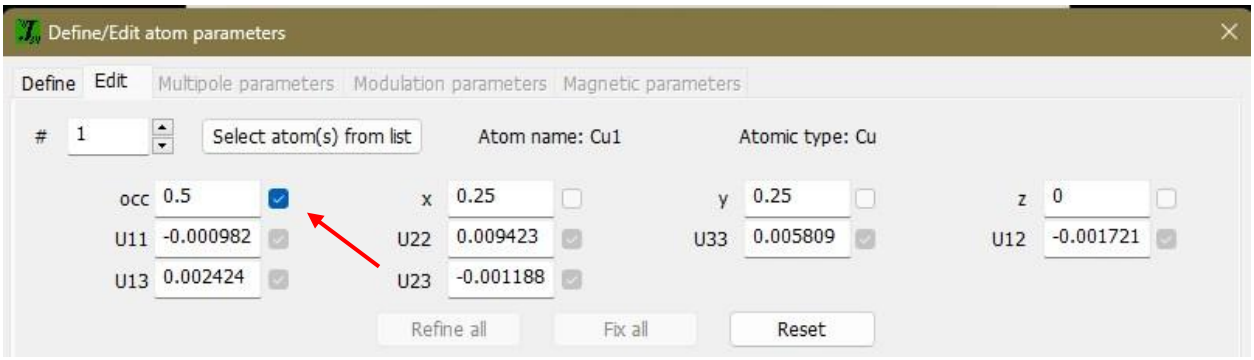
All refinable parameters are divided into two groups: *automatic* and *user-controlled* ones. The automatic parameters are those which can be usually refined without numerical problems: scale factors and extinction parameters; parameters describing position, ADP and their modulation for individual atoms as well as for molecules; background parameters of the powder profile; magnetic parameters. The user-controlled parameters are twin/phase volume fractions, atomic or molecular site occupancies, parameters of crenel modulation functions, parameters of multipole refinement and powder profile parameters for individual Bragg reflections.

The automatic parameters are activated by default at the beginning of the refinement process while the user-controlled ones must be always explicitly activated by the user. The program always fixes the parameters which cannot be refined due to symmetry restrictions. In order to fix other automatic parameters the user is provided with a range of special fixing commands. This way is very useful for most cases because it minimizes mistakes in setting refinement flags. However the program also allows switching to a completely manual mode, where all parameters are to be activated explicitly by the user, analogically like in other refinement programs such as FullProf [29].

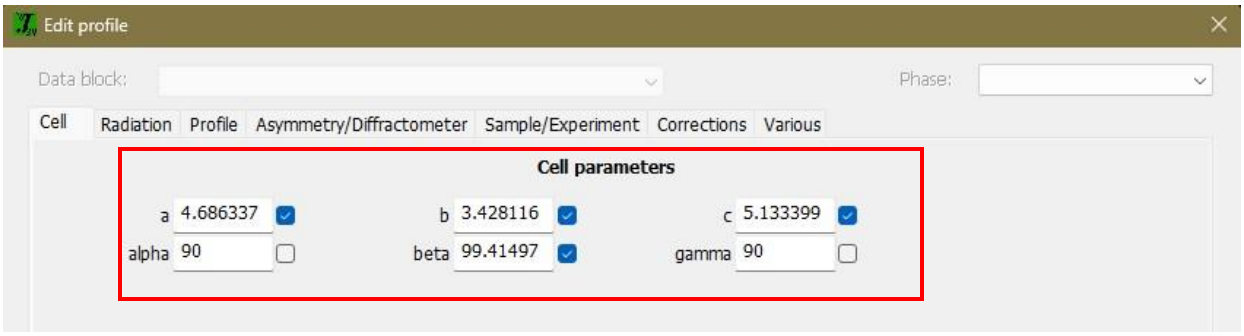
In the last several versions of Jana2020, we decided to prevent the selection of refinement keys for automatic keys. This is demonstrated in the following dialogs:

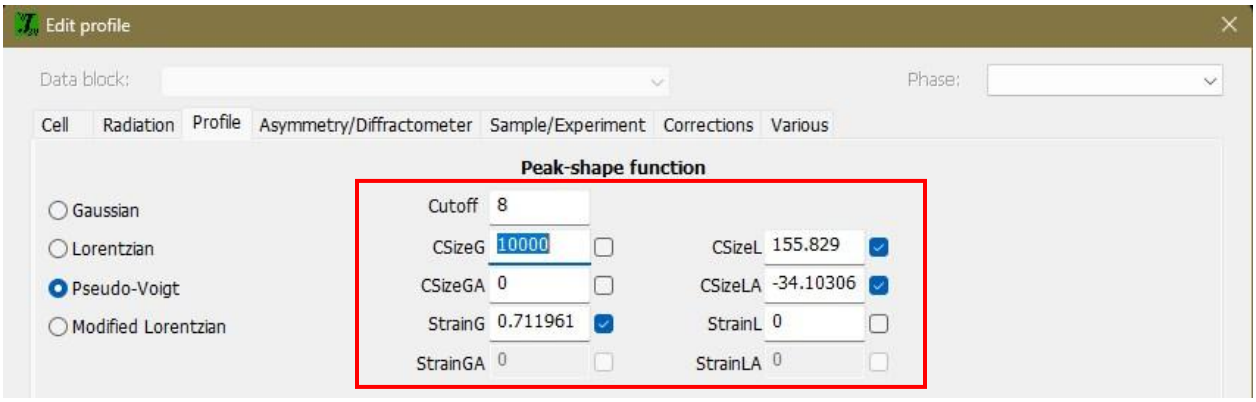


The automatic keys are highlighted in green, and the user-controlled ones are in red.

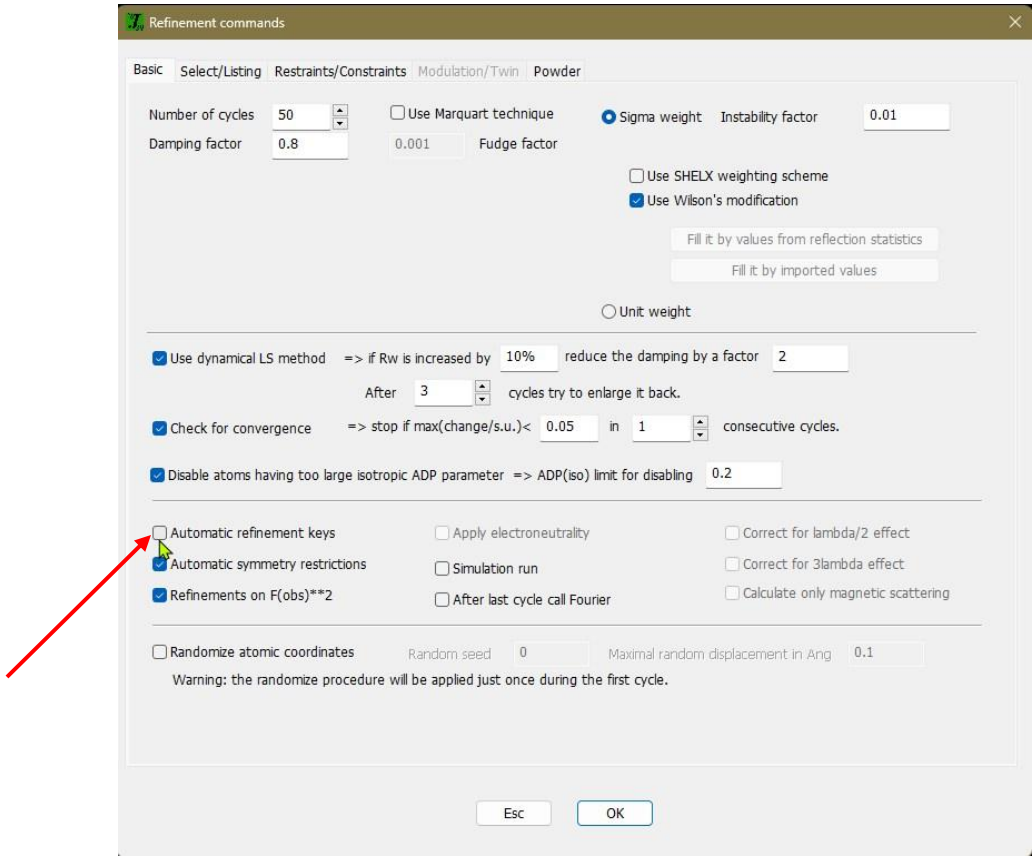


For the powder parameters, all refinement keys are user-controlled:





In the refinement dialog, you can switch off the automatic procedure:



Then, the user must decide which parameters to refine and which not: