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CCP14

Tutorials and Examples

Powder Cell for Windows, Structure Visualisation/Manipulation, Powder Pattern Calculation and Profile Fitting by Werner Kraus and Gert Nolze

Basic Runthrough demonstration of Powder Cell

The CCP14 Homepage is at ***http://www.ccp14.ac.uk***

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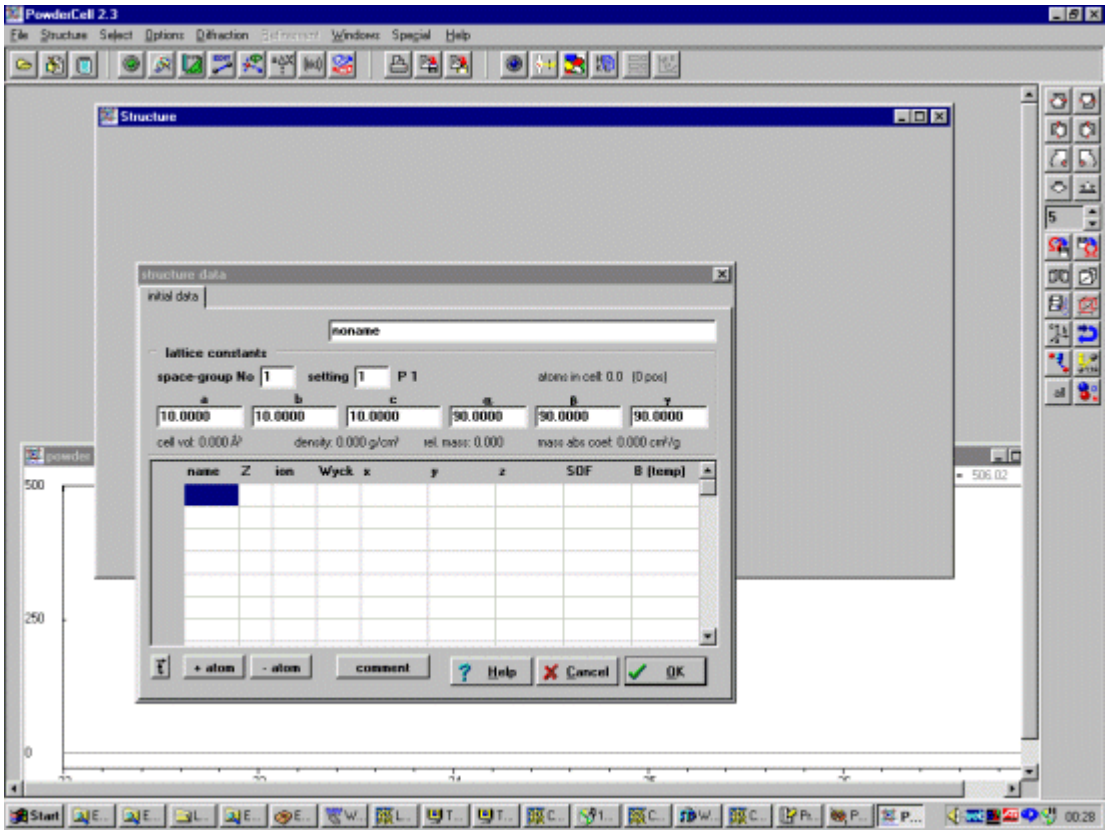
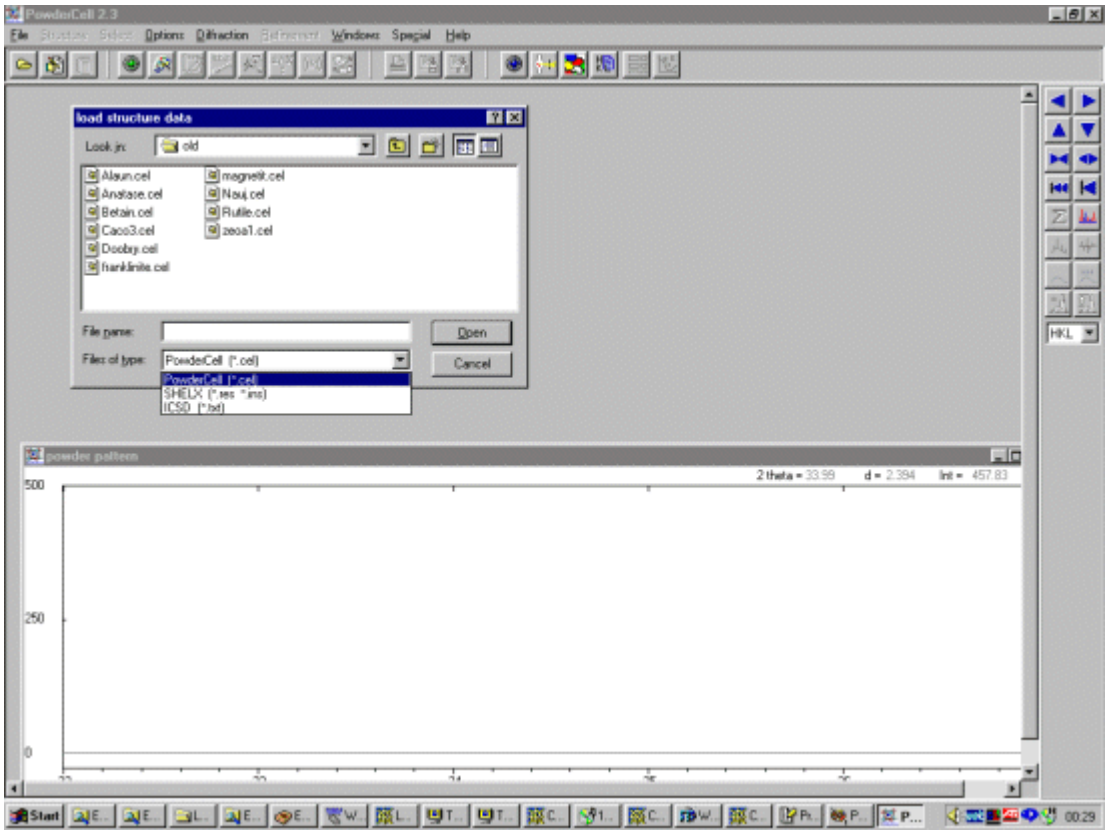
The following run-through is for Powder Cell 2.3

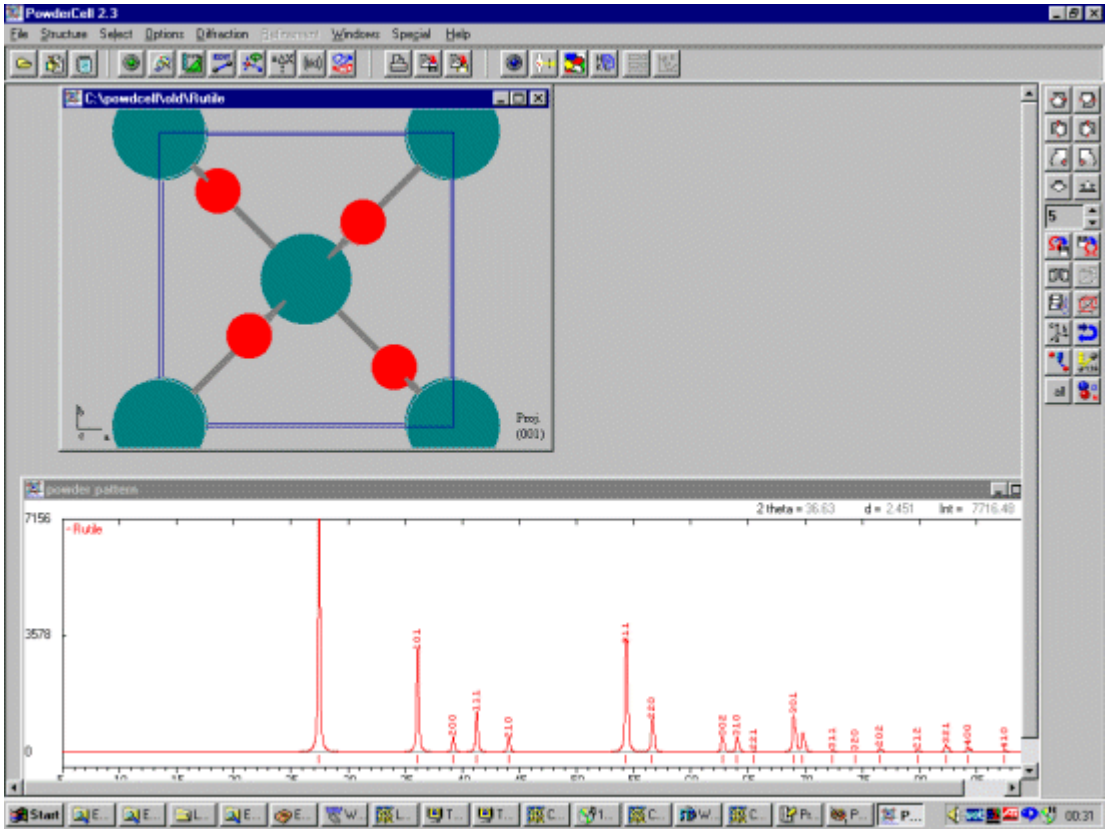
If you enter a new structure from scratch with Powder Cell by selecting **File, New**, input is done via a menu interface.



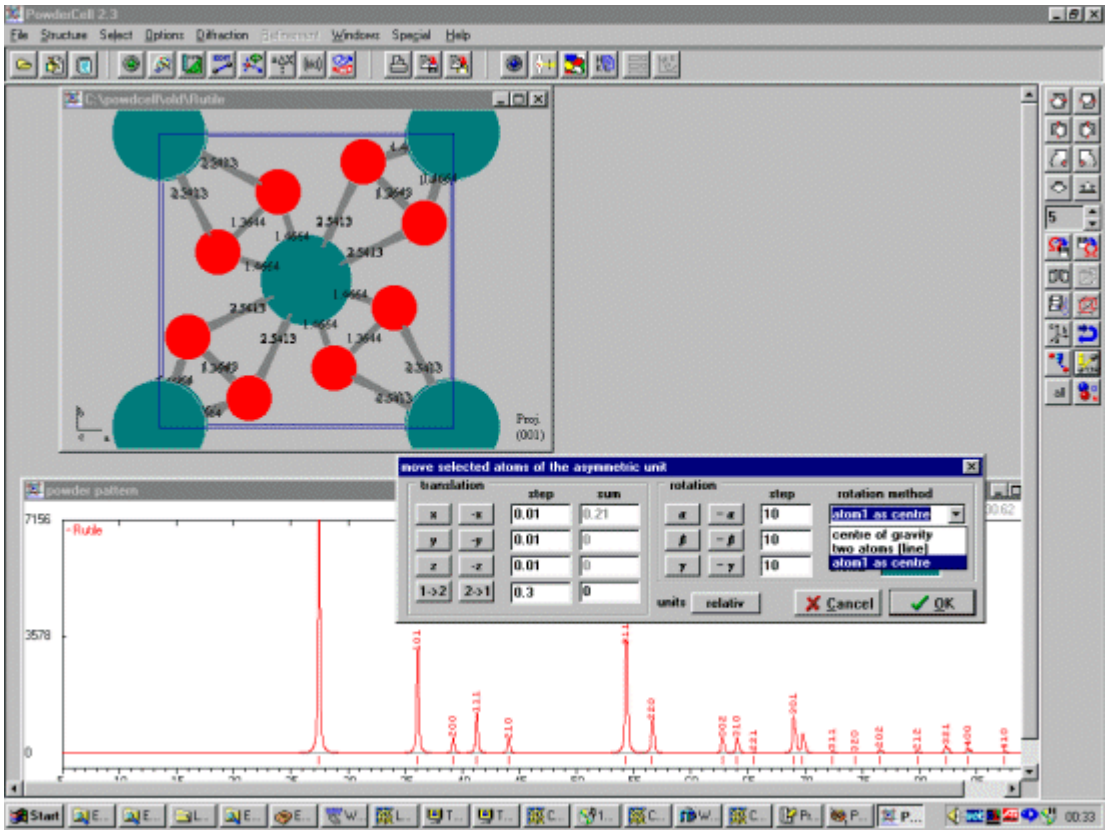
Otherwise, Shelx and ICSD files can be used by selecting **File, Load**.



Once a file is selected or a new crystal structure is inputted, Powder Cell will draw the structure and depending on the saved defaults, calculate a Powder pattern. Multiple crystal structures can be opened, which can then be used to explore quantitative analysis and multiphase mixtures.

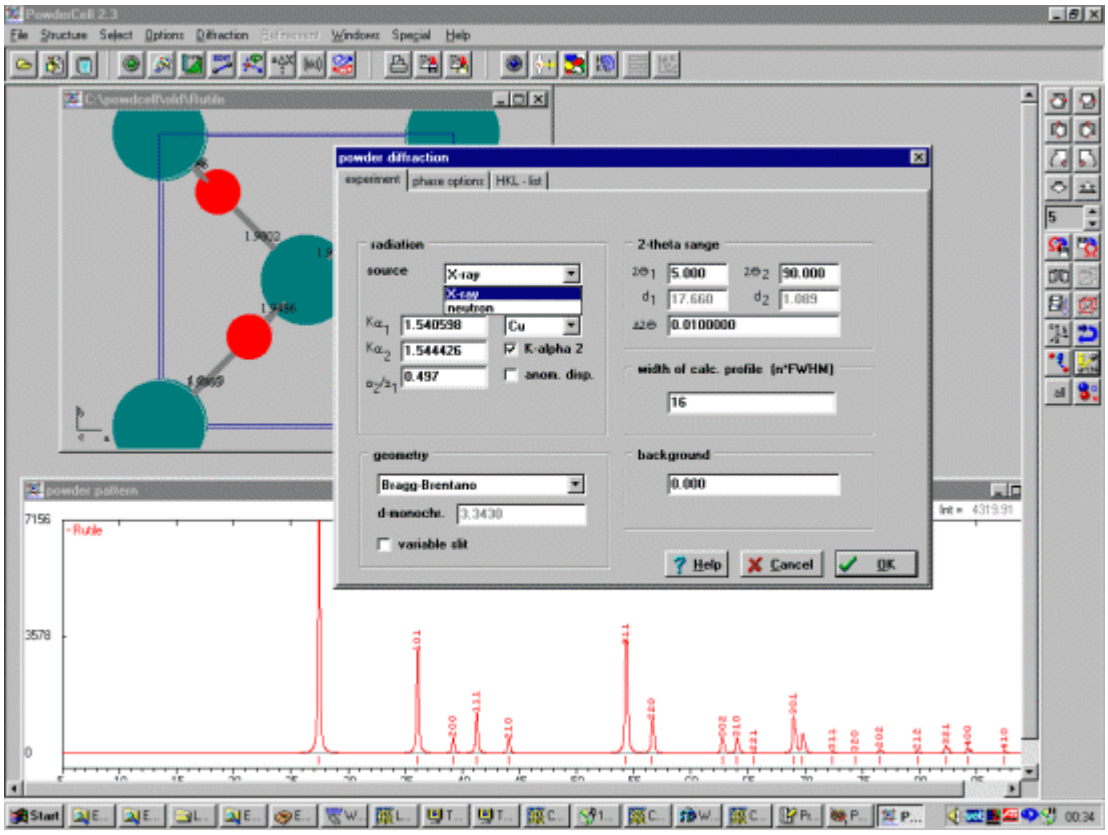


Individual or groups of atoms can be selected via the **Select** menu, and moved around via the menu interface **(Select, Move Selected Atoms)**; with new powder patterns being calculated on request. The user has the option to display Bond-lengths on the screen at all times.

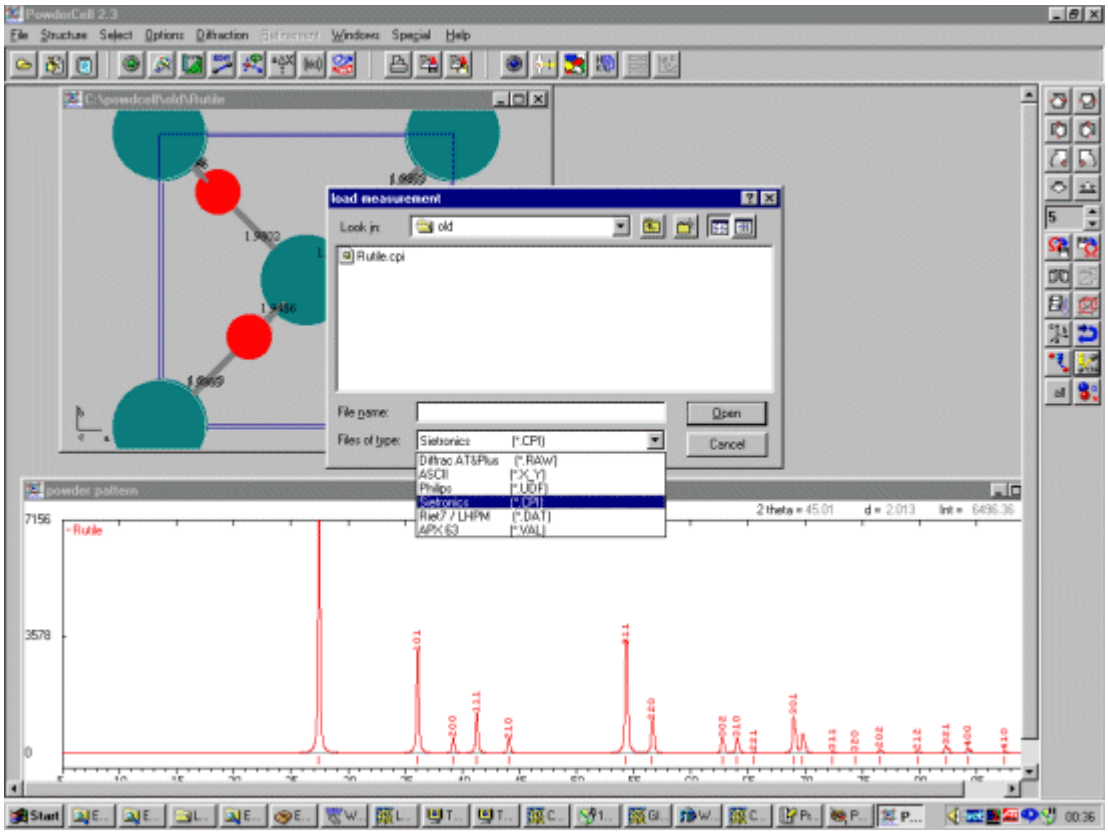


Phase transitions can be explored using the **Structure, Subgroups**, **Structure, Super Groups** menu options. This takes into account all the symmetry requirements of performing such an operation.

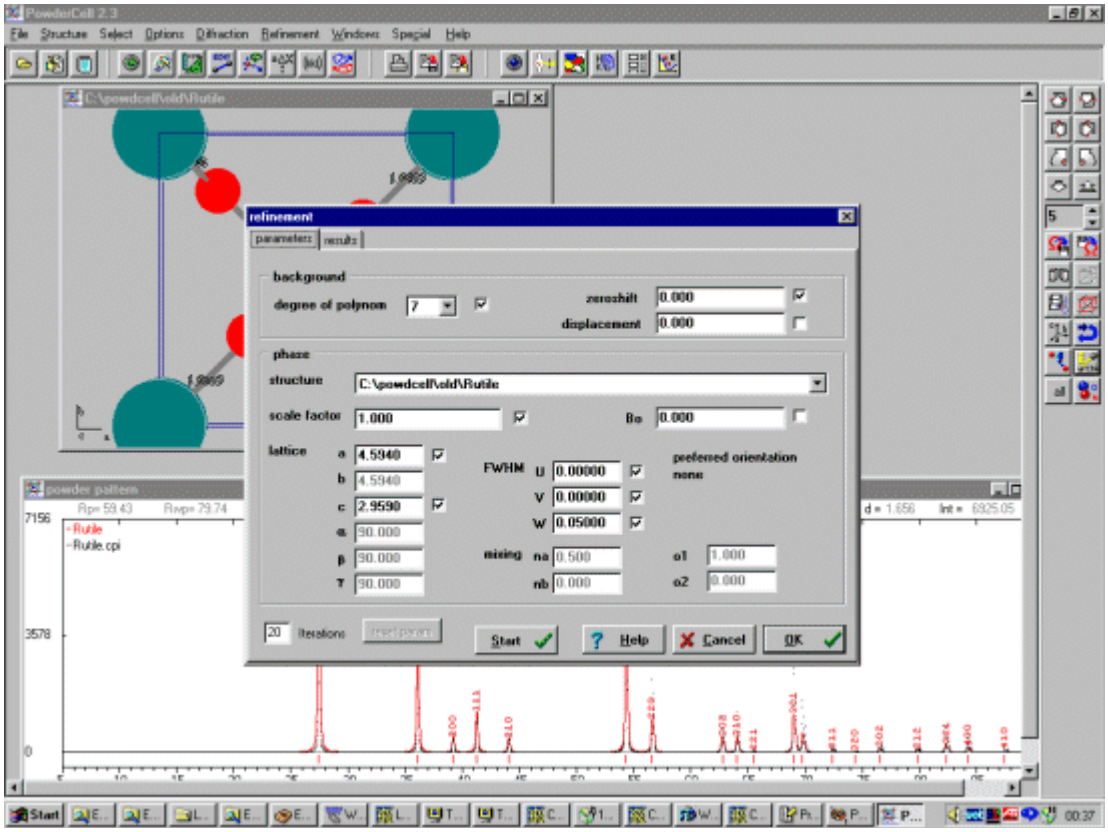
Neutron and X-ray patterns can be calculated; then saved in a variety of formats including CPI and Siemens/Burker format using the **Diffraction, Export Data** menu.



To aid in trialing structures and exploring phase transitions and structure modifications; it is possible to import "raw diffraction data" in a variety of data formats.

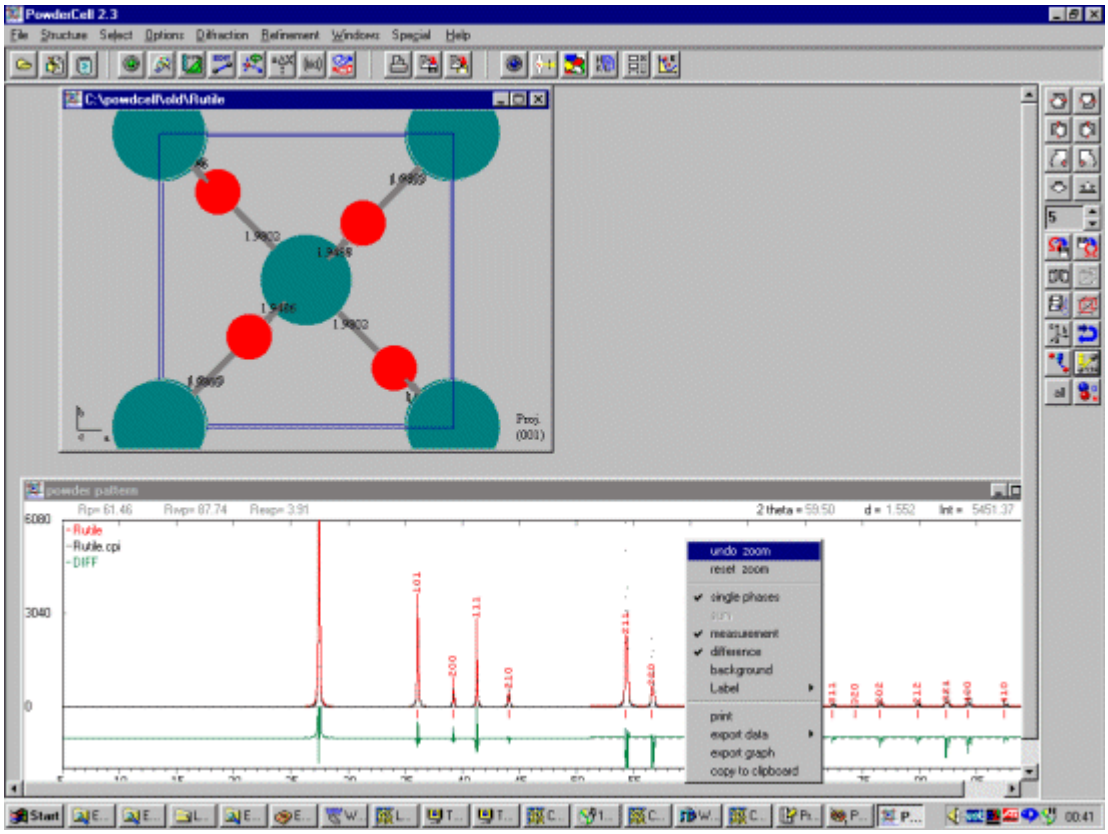


The unit cell and width/shape of the opened crystal structures can then be fitted to the raw diffraction data by using the **Refinement** menu options.

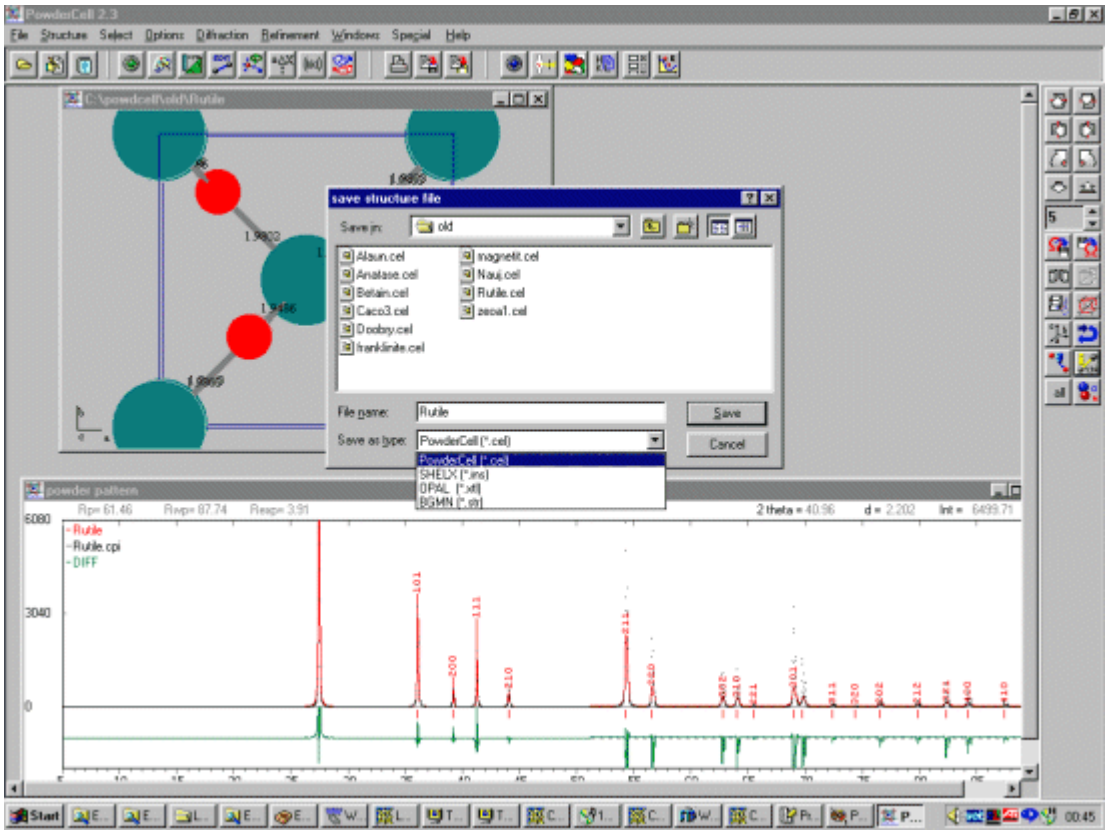


It is possible to enhance the display such as providing a plot of the difference in the fit. While you have the powder pattern window selected, click on the right mouse button to see a list of configurable options.

Once you have fitted/refined the cell and width/shape; you can continue trying model structures/changing your structure and seeing how it matches the raw diffraction data. This can be used to examine how structural changes may affect the pattern. Or Powder Cell can be used in this mode to try and obtain a decent starting structure to refine via a Rietveld refinement program.



For continuation via other structure solution and refinement software, Powder Cell can save the structure into a variety of formats include, Shelx, Opal and BGMN Rietveld | [CCP14 BGMN Mirror].



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If you have any queries or comments, please feel free to contact the CCP14