

Data corrections (DaVinci1 - the routine powder diffractometer)

Description

Unfortunately there is a problem with the goniometer on DaVinci1, meaning that there will be a slight shift of the peaks (it is different for different angles) compared to the database.

How to analyse the data with best possible result

EVA Search and Match (fingerprinting)

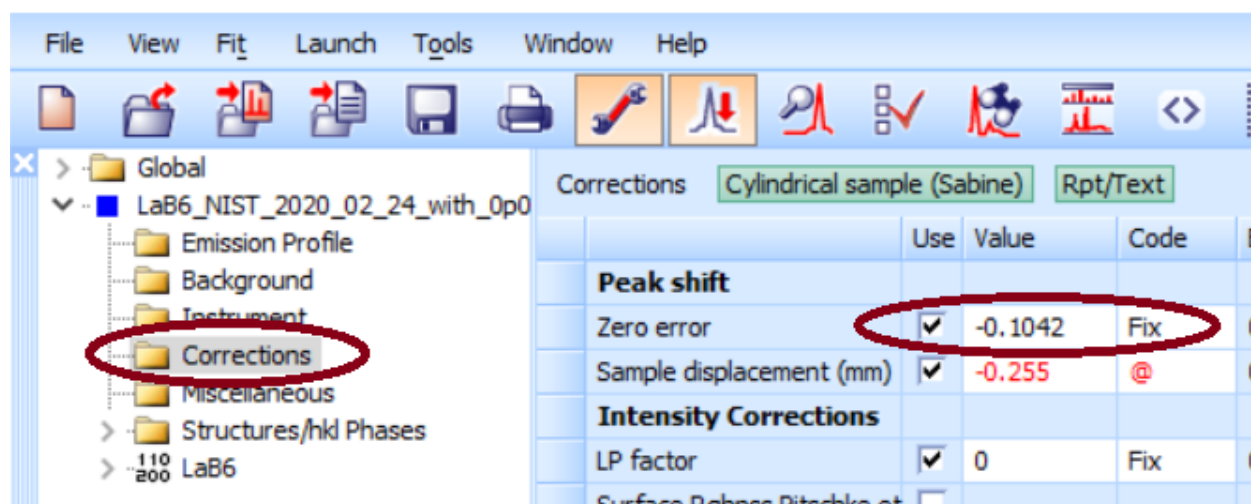
(Still working on it! Sorry for the delay.)

Topas (Pawley and Rietveld fitting)

After importing your data, you need to edit the following fields under "Corrections"

- Zero error = -0.1042 (Fixed)
- Sample displacement: For a perfectly mounted sample, the sample height is approximately -0.2550 mm. However, this value you can refine to fit your sample.

These values have been found by fitting both the measurements of NIST 660a (LaB6) and NIST 1967a (corundum) standards simultaneously.



	Use	Value	Code	E
Peak shift				
Zero error	<input checked="" type="checkbox"/>	-0.1042	Fix	0
Sample displacement (mm)	<input checked="" type="checkbox"/>	-0.255	@	0
Intensity Corrections				
LP factor	<input checked="" type="checkbox"/>	0	Fix	0
Surface Roughness Pitschke et	<input type="checkbox"/>			

Example: How to refine for a LaB6 sample (coated on Si-wafer). Keep Zero error fixed at "-0.1042", whilst refine the sample height.

More details:

Figures illustrating the offsets can be found [here](#).

Relevant links: