INDIAN INSTITUTE OF TECHNOLOGY KANPUR
DEPARTMENT OF CHEMICAL ENGINEERING
PG Research lab

STANDARD OPERATING PROCEDURE
XPERT POWDER (XRD)

Peak Matching in Panalytical XRD Software High Score

A) Importing Data

1. Open HighScore software.
2. Go to File → Open and load the XRD data file (.xrdml).
3. Verify that the intensity vs. 2θ graph appears correctly.

B) Background Subtraction

1. Select "Background" from the menu.
2. Choose an appropriate background model (e.g., Polynomial, Strip, or SNIP).
3. Apply and verify baseline correction.

C) Peak Identification

1. Click "Search Peaks" and adjust sensitivity settings.
2. Manually refine peak positions if necessary.
3. Compare detected peaks with standard reference databases.

D) Phase Identification

1. Open "Identify Phases" and load a reference database.
2. Select a search-match algorithm (e.g., Search-Match, RIR method).
3. Validate phase identification by reviewing peak matches.

E) Peak Fitting and Profile Refinement

1. Use the Peak Fitting Tool for Gaussian/Lorentzian peak fitting.
2. Adjust peak shapes and widths for better fitting.
3. Verify R^2 values to ensure an accurate fit.

F) Rietveld Refinement (if applicable)

1. Import a structure file (.cif or .prf).
2. Set refinement parameters (lattice constants, peak profiles, etc.).
3. Run refinement and check for a low Rwp value (good fit).
4. Make necessary adjustments to improve the refinement.

G) Data Export and Reporting

1. Save the refined dataset (.hpf or .xrdml).
2. Export results in PDF or Excel format.
3. Include phase details, peak lists, and refinement results in the report.