THE BENEFITS OF AN INTEGRATED FULL PATTERN PXRD ANALYSIS APPROACH

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In this presentation we will highlight some advantages of complete analysis integration as available in our new full pattern PXRD analysis software: X’Pert HighScore Plus V2.2. This package not only includes phase identification, Rietveld analysis and indexing, but it also offers a great variety of pattern treatment methods together with different kinds of high throughput methodologies like agglomerative cluster analysis, principal component analysis, fuzzy clustering and more. Further all major current XRD databases are supported and can be accessed via one convenient user interface. For example, this allows fully automatic phase identification with subsequent quantitative Rietveld analysis with just one click of a button.

All treatment methods, analysis techniques, and the reporting are seamlessly integrated into a 21 CFR Part 11 support mode compliant, MS Office XP® like user interface. This offers standard convenience functionality like multiple step Undo/Redo, clipboard/print preview support or document based operation. All functions can easily be automated. For the advanced user who requires total freedom of use, the complete document object model is published and can be exploited by calling standard PASCAL scripts in user batches.

The benefits of this 'complete X-ray powder pattern analysis solution' are demonstrated with a few everyday application examples, ranging from Rietveld-based quantitative phase analysis to crystallinity determination, non-ambient analysis, detection of outliers and high throughput data evaluation.