Display and Capabilities

PDF-4+   **PDF-4+/Web**   **PDF-4/Axiom**   **PDF-4/Minerals**   **PDF-4/Organics**   **PDF-2**

ICDD's data mining software provides display, search and data mining choices with display fields that work interactively with our searches. Graph and plot your data, simulate diffraction patterns, search by subfile, and explore more data filtering capabilities.

*PDF-4/Sleve+ only

Search Results
- User-selectable display fields
  - Color coded quality marks
  - Formula and nomenclature fields
  - Strongest and longest lines
  - Unit cell data
  - Atomic coordinates flag*
  - And many more…
- All fields can be sorted
- Calculations for all numeric fields (mean, median, and ESD)
- User-defined graphing of most fields (x-y graphs, histograms, and category graphs)

PDF Card
- d-spacing table and graph for fixed slit intensity, variable slit intensity, and integrated* intensity
- Simulated diffraction pattern*
- Formula and nomenclature fields
- Temperature of data collection
- Unit cell data
- Cross referenced atomic coordinates*
- Crystal (Symmetry Allowed) data field
- References table with DOI's (Digital Object Identifiers)
- XML export

Simulated Diffraction Patterns*
- X-ray diffraction, neutron diffraction, and electron diffraction
- Bragg-Brentano or Debye-Scherrer geometry
- 2θ zero correction
- 2θ, Q, d, and 1/d options for x-axis
- Linear, logarithmic, and square root intensity options for y-axis
- JPEG, PNG, and TIF exports

Raw diffraction (PD3) patterns*

Temperature series *

ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

ISO 9001:2015
QUALITY MANAGEMENT SYSTEM CERTIFIED
BY DEKRA

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Display and Capabilities (continued)

▶ **2D structure diagrams**

▶ **3D molecular structures***

▶ **Bond lengths/angles display***

▶ **Selected Area Electron Diffraction (SAED) patterns***
- Overlay image for visual comparison and spot indexing

▶ **Electron Backscatter Diffraction (EBSD) patterns***

▶ **Ring patterns***
- Overlay image for visual comparison
- Option to simulate uniaxial preferred orientation
- Area detector and strip detector simulations

▶ **Total pattern analysis*:** Similarity index compares imported experimental data to simulated diffraction patterns

▶ **Sleve/Sleve+**
- Phase identification plugin
- Automatically import experimental data for all major XRD file types
- Support for importing 2D diffraction (ring) patterns from image files for visual analysis*
- Custom data processing sets for background removal, smoothing, $K\alpha2$ stripping, and peak finding
- Semi-quantitative analysis using RIR method*
- "Smart I/Ic Substitution" uses dynamically cross referenced I/Ic values*

▶ **Microanalysis Search -** Allows the user to search the database using elemental composition obtained from a micro-XRF analysis, microprobe analysis, or other elemental analysis.

▶ **Composition Graph -** Allows the user to search the database and group binary and ternary PDF entries based on their composition values (atomic percent or weight percent).