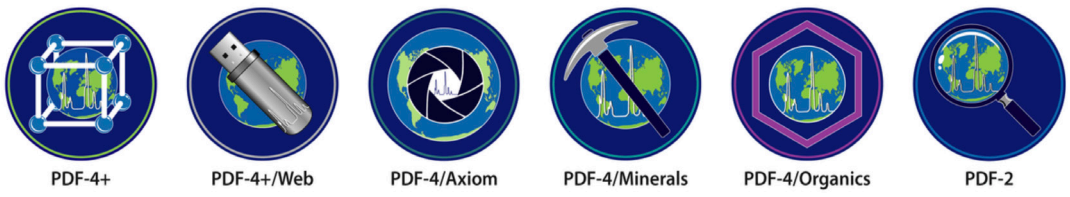
Data Mining Searches & Display and Capabilities



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.

Data Mining Searches

Database filters:

- Subfiles:
  - Cement & hydration product
  - Metals & alloys
  - Mineral related
  - Organics
  - And many more...
- Environment conditions (ambient or non-ambient temperature/pressure)
- Has atomic coordinates*
- Has raw diffraction (PD3) patterns*
- Database status (primary, alternate, or deleted)
- Quality mark

Periodic table

- Boolean searches
- Yes/no/maybe searches
- composition list

Chemistry searches:

- Formula (chemical, empirical, structural, or refined)
- Name (compound, mineral, common, or zeolite)
- IMA number
- CAS number
- Number of elements
- Molecular weight
- Composition (weight % or atomic %)

Classification searches:

- Mineral classification
- Zeolite classification
- Organic function group
- Pearson symbol (with or without hydrogen)
- Construct pearson symbol (crystal system, lattice centering, and atomic count)
- Prototype structure (chemical formula order or alphabetical order)
- Formula type (anx)
- Wyckoff sequence

Crystallography searches:

- Crystal system
- Crystal (centrosymmetric or non-centrosymmetric)
- Atomic environment type*
- Space group:
  - Space group symbol
  - Space group number
  - Aspect symbol
  - Superspace group symbol
- Unit cell (axis, axial ratio, and volume)
  - Crystal data
  - Reduced cell
  - Author's cell
  - Supercell/subcell

Modulated structure searches

- Modulated dimension
- Number of subsystems

Diffraction searches

- Strong line (D1, D2, D3) – X-ray or neutron diffraction*
- Long line (L1, L2, L3) – X-ray or neutron diffraction*
- Reported intensity
- I/I-corundum – X-ray or neutron diffraction*
- R-factor
- Smith-snyder figure of merit
- Temperature of data collection
- Pressure of data collection

Physical property searches

- Melting point
- Density (measured, calculated, and structural)
- Color
- Has property sheet*
- Has topology data*
- Topology*

***PDF-4 only**

Reference searches
- Author
- Title
- Publication (journal or coden)
- Volume
- Year
- DOI (digital object identifier)

Database comments search

Display and Capabilities

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 *

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

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

SIeve/SIeve+
- 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, Kα2 stripping, and peak finding
- Semi-quantitative analysis using RIR method*
- "Smart I/Ic Substitution" uses dynamically cross referenced I/I_c 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).

***PDF-4/SIeve+ only**

Celebrating 80 years 1941–2021 ICDD® International Centre for Diffraction Data

ISO 9001:2015 QUALITY MANAGEMENT SYSTEM CERTIFIED BY DEKRA CERT. NO. 110409.01

@TheICDD @TheICDD @ICDDICDD @TheICDD