

Data Mining Searches



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.

► Database filters:

*PDF-4 only

- 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, alternate, 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



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▶ **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*
 - Volume
 - Surface area
 - Total porosity

▶ **Reference searches**

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

▶ **Database comments search**



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