

Data Mining Searches

▶ 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

▶ Chemistry Searches:

- Formula (chemical, empirical, structural, or zeolite)
- Formula Type (ANX)
- Name (compound, mineral, or common)
- Composition (weight % or atomic %)
- Number of Elements
- Molecular Weight
- Mineral Classification
- Zeolite Classification
- Organic Function Group

▶ Crystallography Searches:

- Space Group:
 - Space Group Symbol
 - Space Group Number
 - Aspect Symbol
- Pearson Symbol (with or without hydrogen)
- Construct Pearson Symbol (crystal system, lattice centering, and atomic count)
- Atomic Environment Type*
- Prototype Structure (chemical formula order or alphabetical order)
- Unit Cell (axis, axial ratio, and volume)
 - Crystal Data
 - Reduced Cell
 - Author's Cell
 - Supercell/Subcell
 - Crystal (centrosymmetric or non-centrosymmetric)

▶ 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*
- I/I-corundum – X-ray or Neutron Diffraction*
- R-factor
- Smith-Snyder Figure of Merit
- Temperature of Data Collection

▶ Physical Property Searches

- Melting Point
- Density (measured, calculated, and structural)
- Color
- Has Topology Data*
- Has Property Sheet*

▶ Reference Searches

- DOI (digital object identifier)
- Title
- Author
- Publication (journal or CODEN)
- Volume
- Year
- CAS Number

▶ Database Comments Search