

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, or structural)
 - Formula Type (ANX)
 - Name (compound, mineral, or common)
 - Composition (weight % or atomic %)
 - Number of Elements
 - 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 Property Sheet*
- ▶ **Reference Searches**
 - DOI (digital object identifier)
 - Title
 - Author
 - Publication (journal or CODEN)
 - Volume
 - Year
 - CAS Number
- ▶ **Database Comments Search**