

PDF-2 Tools and Searches



PDF-2 2018

The PDF-2 2018 database is powered by our integrated search display software. PDF-2 2018 boasts 68 search selections coupled with 53 display fields resulting in a nearly limitless choice of data mining options. This quick tutorial will introduce you to the basics of PDF-2 filters available to you to refine your search.

Getting Started: The Toolbar

Search Window: Overview of Search Classifications

Data Mining Basics

Search Example

PDF Data Card

Launch Screen

This will be the opening screen when you have correctly opened PDF-2 2018.

PDF-2 2018

File Edit Window Help

Open PDF Cards Preferences Search History Results Sieve Microanalysis

Search

Subfile

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Boolean Search ☒ Yes/No/Maybe Search

Set Unselected to No

Search

Reset Tab

Reset All

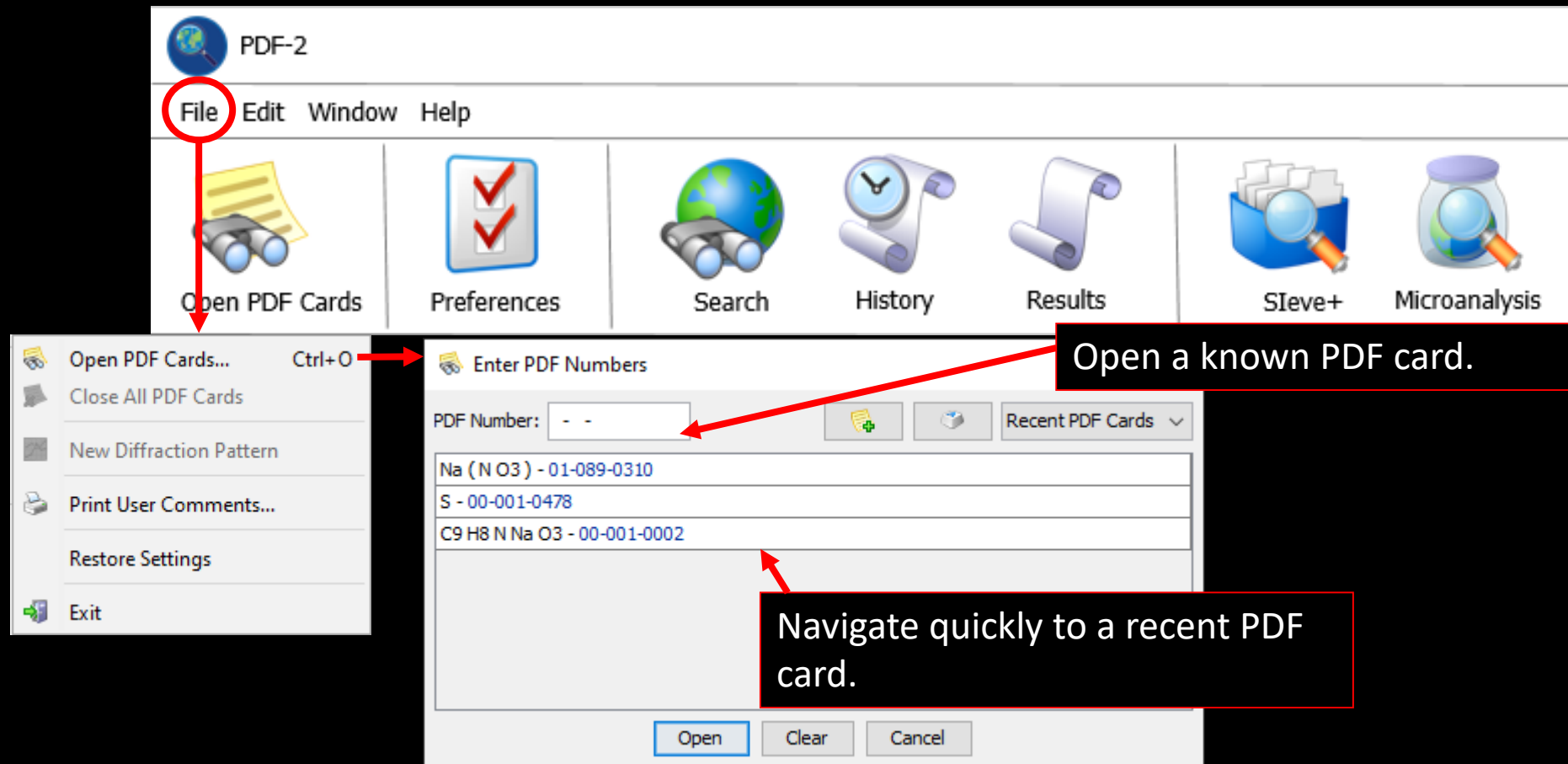
Help

Numeric Input Global Operator

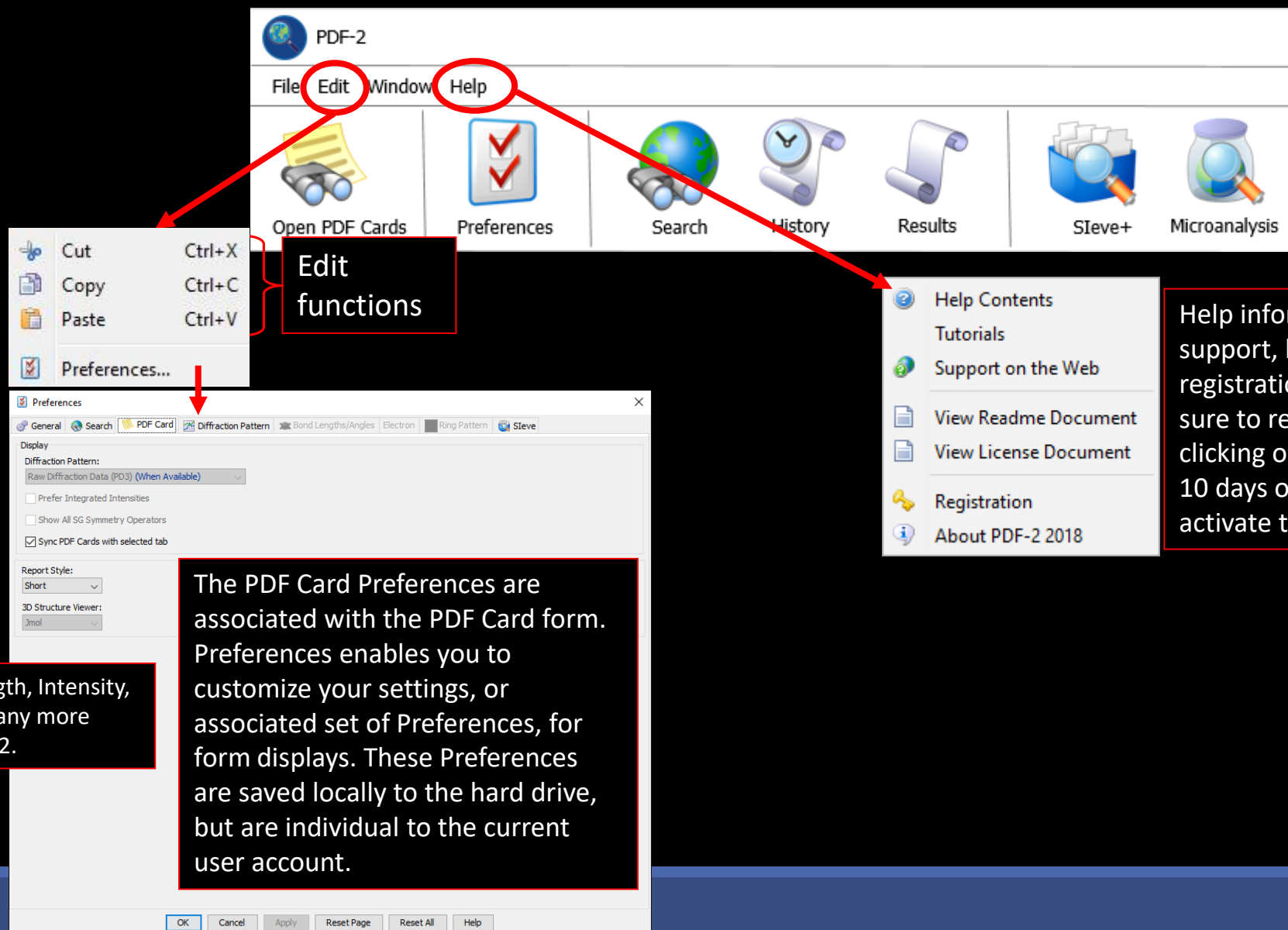
Tool Bar

Primary Search Menu

Getting Started



Getting Started



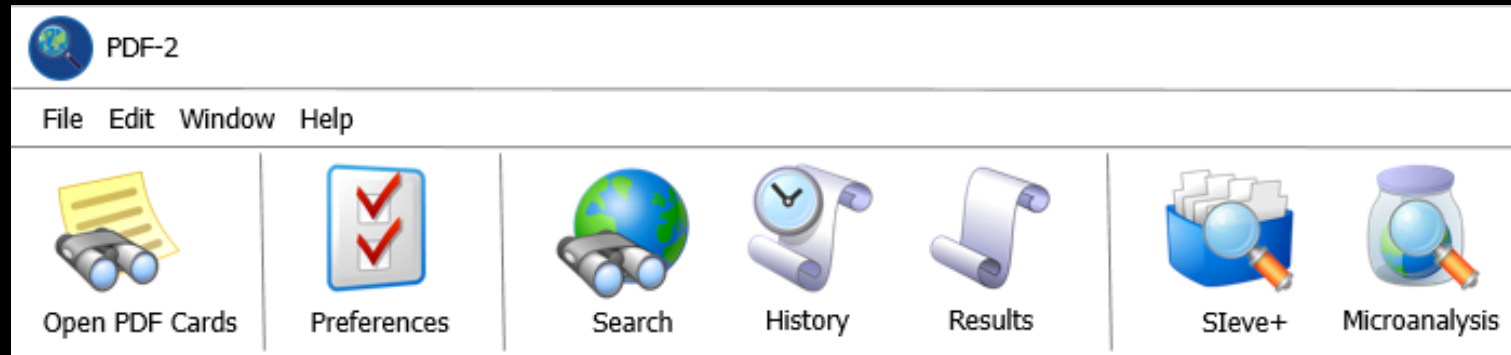
Edit functions

Help information regarding use, support, license policy, and registration of the PDF-2. Be sure to register the PDF-2 by clicking on Registration within 10 days of installation to activate the full license term.

The PDF Card Preferences are associated with the PDF Card form. Preferences enables you to customize your settings, or associated set of Preferences, for form displays. These Preferences are saved locally to the hard drive, but are individual to the current user account.

Customize Wavelength, Intensity, Report Style, and many more features of the PDF-2.

Tool Bar



Quick Navigation Icons



Select a PDF Card



Select Preferences Module



Open Search Window



Microanalysis



Open History Window



Open Results Window



Open Sieve

Primary Search Menu

The Search Window displays nine tabs. Each tab features multiple search criteria to allow you to data mine the PDF-2. Searching the PDF-2 is an iterative process that allows you to input user-defined criteria, view the results, and combine additional criteria to refine your results.

The screenshot displays the 'Search' window with the following sections:

- Subfile:** Custom PDF Set (Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial).
- Environment:** Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary, Alternate, Deleted.
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).
- Periodic Table:** A table with columns IA through VIIIA and rows 1 through 7. Elements are color-coded by group.
- Search Options:** Boolean Search (radio buttons), Yes/No/Maybe Search (radio buttons), And/Or/Not (radio buttons), Grouping (radio buttons).
- Search Bar:** Search, Reset Tab, Reset All, Help.
- Input Fields:** Numeric Input, Global Operator.

Search Window

Subfiles/Database Filters

Search

Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Boolean Search ☒ Yes/No/Maybe Search ☐

And ☐ Or ☐ Not ☐

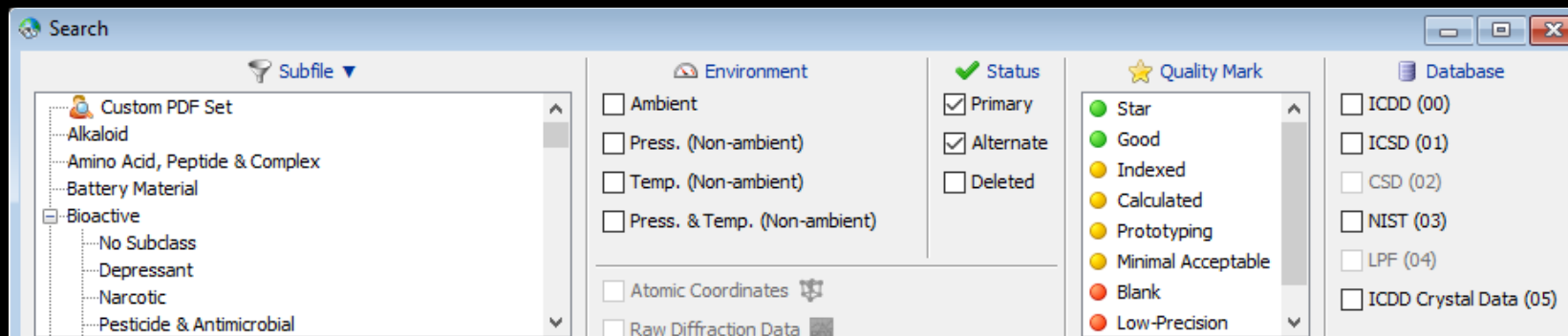
Grouping: ☐ And ☐ Or

Refine your search by selecting filters.
Select criteria under **Subfile**, **Environment**,
Status, **Quality Mark (QM)**, and **Database**.

Search Reset Tab Reset All Help Numeric Input ▼ Global Operator ▼

Search Window

Subfiles/Database Filters



Filters:

Subfile – select filters related to assigned subfiles/subclass.

Environment – select filters related to the environment (especially temperature and pressure).

Status – select filters based on the status of the pattern, which can be Primary, Alternate, or Deleted.

Quality Mark (QM) – select filters related to the quality evaluation assigned to the data.

Database – search the entire database or select the data entry source (i.e., ICDD (00) – ICDD's experimental patterns).

Search Window

Periodic Table Filters

The screenshot displays the ICDD Search Window interface. At the top, there are tabs for 'Subfile', 'Environment', 'Status', and 'Quality Mark'. The 'Subfile' tab is active, showing a tree view of 'Custom PDF Set' with categories like Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial. The 'Environment' tab has checkboxes for Ambient, Press. (Non-ambient), Temp. (Non-ambient), and Press. & Temp. (Non-ambient). The 'Status' tab has checkboxes for Primary, Alternate, and Deleted. The 'Quality Mark' tab has a list of quality marks: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision. Below these tabs is a 'Periodic Table' section with a grid of elements. The elements are color-coded by group: IA (green), IIA (blue), IIIB (purple), IVB (orange), VB (red), VIB (yellow), VIIB (light green), VIIIB (pink), IB (light blue), IIB (light green), IIIA (light blue), IVA (light green), VA (light blue), VIA (light green), and VIIA (light blue). The periodic table is organized into rows and columns, with elements labeled by their atomic number, symbol, and name. A red arrow points to the 'Boolean Search' section, which includes radio buttons for 'And', 'Or', and 'Not', and a 'Grouping' section with radio buttons for 'And' and 'Or'. The 'Boolean Search' section also includes a text input field for the search criteria. The 'Periodic Table' section includes a 'Formula/Name' input field and a 'Classifications' section with a list of categories: Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial. The 'Periodic Table' section also includes a 'Crystallography' section with a list of categories: Modulated, Diffraction, Physical Properties, Reference, and Comments. The 'Periodic Table' section includes a 'Comments' section with a text input field for the search criteria. At the bottom of the window, there are buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help'. There is also a 'Numeric Input' section with a dropdown menu for 'Global Operator' and a text input field for the search criteria.

Refine your search by selecting filters based upon the elements in a material. Select elements individually (i.e., *H*, *He*, *Li*, etc.) or by group (i.e., *IA*, *Noble Gases*, *Period 1*, etc.).

Select the *Inner Operator* to combine the elements in the group using *Not*, *And*, *Or*, *Only* and *Just*.

Select the *Outer Operator* to combine element groups using *And* & *Or*.

Search Window

Periodic Table Filters

[illegible]

For the **Yes/No/Maybe** search, click an element to cycle through these three states:

Yes - This element must exist in the pattern (white)

No - This element must not exist in the pattern (black)

Maybe - This element may exist in the pattern (colored)

Search Window

Formula/Name

- Any Formula
- Chemical Formula
- Empirical Formula
- Structural Formula
- Contains Elements
- Contains Phrase
- Exactly
- Not

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Formula ▼

Any Formula

Name ▼

Any Name

IMA No.

CAS Number

Number of Elements Low High

Composition ▼

Element Weight % ESD

Search Reset Tab Reset All Help Numeric

Refine your search by selecting filters based upon the elements in a material.

Chemical Formula – filters based on the molecular formula.

Empirical Formula – filters on an element that has a particular atom count as expressed in the formula.

Structural Formula – filters on the chemical formula that shows how atoms are bonded to one another in a molecule.

Number of Elements – filters on the total number of unique elements in a chemical formula.

Composition – filters on the weight percent or atomic percent of the formula.

Search Window

Formula/Name

The screenshot shows the ICDD Search Window with the following sections:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (expanded), No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial.
- Environment:** Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary, Alternate, Deleted.
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).
- Search Criteria:** Formula (Any Formula), Name (Any Name), IMA No., CAS Number, Number of Elements (Low to High), Composition (Element, Weight %).
- Left Panel:** Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, Comments.

Refine your search by selecting filters based upon the name or name fragment of a material.

Compound Name – filters based on the compound name.

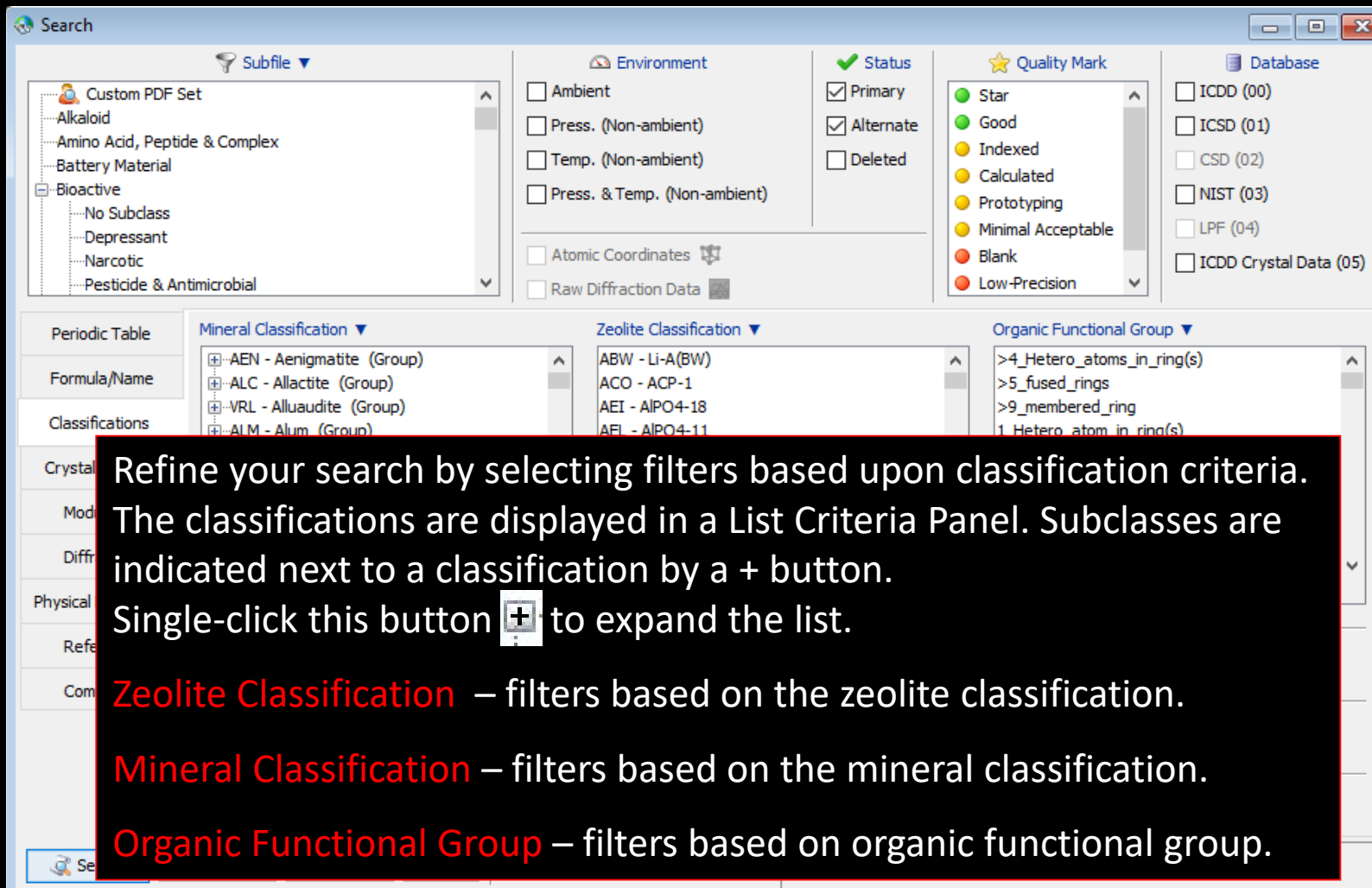
Mineral Name – filters based on the mineral name.

Alternate Name – filters based on another recognized name of the material.


- Any Name
- Compound Name
- Mineral Name
- Alternate Name
- Contains Fragments
- Contains Phrase
- Exactly
- Not

Search Window

Classifications



The screenshot shows the ICDD Search Window with several filter panels. The 'Subfile' panel on the left lists categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The 'Environment' panel includes checkboxes for 'Ambient', 'Press. (Non-ambient)', 'Temp. (Non-ambient)', and 'Press. & Temp. (Non-ambient)'. The 'Status' panel has checkboxes for 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' panel features a color-coded list: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (red), and Low-Precision (red). The 'Database' panel lists 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'. Below these are three classification panels: 'Mineral Classification' (listing AEN - Aenigmatite, ALC - Allactite, VRL - Alluaudite, and ALM - Alum), 'Zeolite Classification' (listing ABW - Li-A(BW), ACO - ACP-1, AEI - AlPO4-18, and AEI - AlPO4-11), and 'Organic Functional Group' (listing >4_Hetero_atoms_in_ring(s), >5_fused_rings, >9_membered_ring, and 1_Hetero_atom_in_ring(s)). A red box highlights the text explaining how to refine searches using these filters.

Refine your search by selecting filters based upon classification criteria. The classifications are displayed in a List Criteria Panel. Subclasses are indicated next to a classification by a + button. Single-click this button  to expand the list.

Zeolite Classification – filters based on the zeolite classification.

Mineral Classification – filters based on the mineral classification.

Organic Functional Group – filters based on organic functional group.

Search Window

Pearson Symbol Code

The screenshot displays the ICDD Search Window interface. The window is titled "Search" and contains several sections for filtering search results:

- Subfile:** A tree view showing categories like Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial.
- Environment:** Checkboxes for Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, and Raw Diffraction Data.
- Status:** Checkboxes for Primary, Alternate, and Deleted.
- Quality Mark:** A list of quality marks including Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision.
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05).
- Periodic Table:** A sidebar with tabs for Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments.
- Mineral Classification:** A list of mineral groups including AEN - Aenigmatite (Group), ALC - Allactite (Group), VRL - Alluaudite (Group), ALM - Alum (Group), ALN - Alunite (Supergroup), AMB - Amblygonite (Group), AMP - Amphibole (Family), ANC - Analcime (Supergroup), ANY - Ancyrite (Supergroup), ADA - Andalusite (Group), and ANT - Antlerite (Group).
- Zeolite Classification:** A list of zeolite groups including ABW - Li-A(BW), ACO - ACP-1, AEI - AIPO4-18, AEL - AIPO4-11, AEN - AIPO-EN3, AET - AIPO4-8, AFG - Afghanistan, AFI - AIPO4-5, AFN - AIPO-14, AFO - AIPO4-41, and AFR - SAPO-40.
- Organic Functional Group:** A list of organic functional groups including >4_Hetero_atoms_in_ring(s), >5_fused_rings, >9_membered_ring, 1_Hetero_atom_in_ring(s), 1,2_dione____O=C-C=O, 2_fused_rings, 2_Hetero_atoms_in_ring(s), 3_fused_rings, 3_Hetero_atoms_in_ring(s), and 3_membered_rinn.
- Pearson Symbol:** A dropdown menu with "With Hydrogen" selected.
- Prototype Structure:** A text input field with "Any Prototype Structure" and a dropdown arrow.
- Formula Type (ANX):** A text input field with a dropdown arrow.

At the bottom of the window, there are buttons for Search, Reset Tab, Reset All, and Help, along with a Numeric Input field and a Global Operator dropdown.

Filters for Pearson Symbol Codes with and without Hydrogen.

Filters based on a user-constructed Pearson Symbol Code.

Search Window

Crystallography

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☒ Indexed
- ☒ Calculated
- ☒ Prototyping
- ☒ Minimal Acceptable
- ☒ Blank
- ☒ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

- ☐ Tridinic (Anorthic)
- ☐ Rhombohedral
- ☐ Monoclinic
- ☐ Hexagonal
- ☐ Orthorhombic
- ☐ Cubic
- ☐ Tetragonal

Crystal (Symmetry Allowed) ▼

- ☐ Centrosymmetric
- ☐ Non-centrosymmetric:
 - ☐ Enantiomorphic
 - ☐ Pyro / Piezo (p)
 - ☐ Optical Activity
 - ☐ Piezo (2nd Harm.)

Atomic Environment Type

| Symbol | Elements |
|--------|----------|
| | |

Space Group ▼

Space Group Symbol

Crystal Data

Axis (Å)

| a | b | c |
|-------|-------|-------|
| Value | Value | Value |
| ESD | ESD | ESD |

Author's Cell

Supercell/Subcell

Volume

| Value | ESD |
|-------|-----|
| | |

The Crystallography tab displays four additional search tabs: *Crystal Data*, *Reduced Cell*, *Author's Cell*, and *Supercell/Subcell*. Refine your search by selecting filters based upon the structure of a material.

Search Window

Crystal Data

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

- ☐ Tridinic (Anorthic)
- ☐ Rhombohedral
- ☐ Monoclinic
- ☐ Hexagonal
- ☐ Orthorhombic
- ☐ Cubic
- ☐ Tetragonal

Crystal (Symmetry Allowed) ▼

- ☐ Centrosymmetric
- ☐ Non-centrosymmetric:
 - ☐ Enantiomorphic
 - ☐ Pyro / Piezo (p)
 - ☐ Optical Activity
 - ☐ Piezo (2nd Harm.)

Atomic Environment Type

| Symbol | Elements |
|--------|----------|
| | |

Space Group ▼

- ☒ Space Group Symbol
- ☐ Space Group Number
- ☐ Aspect Symbol
- ☐ Superspace Group Symbol
- ☐ Contains Fragments
- ☒ Contains Phrase
- ☐ Exactly
- ☐ Not

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Filters based on the space group symbol according to nomenclature defined by the author.

Filters based on the superspace group symbol (for modulated structures only).

Filters based on the international space group numbers (1-230).

Filters based on the aspect symbol according to nomenclature defined by the author.

Search Window

Crystal Data

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Environment

☐ Ambient

☐ Press. (Non-ambient)

☐ Temp. (Non-ambient)

☐ Press. & Temp. (Non-ambient)

☐ Atomic Coordinates

☐ Raw Diffraction Data

Status

☒ Primary

☒ Alternate

☐ Deleted

Quality Mark

- Star
- Good
- Indexed
- Calculated
- Prototyping
- Minimal Acceptable
- Blank
- Low-Precision

Database

☐ ICDD (00)

☐ ICSD (01)

☐ CSD (02)

☐ NIST (03)

☐ LPF (04)

☐ ICDD Crystal Data (05)

Crystal System

☐ Triclinic (Anorthic) ☐ Rhombohedral

☐ Monoclinic ☐ Hexagonal

☐ Orthorhombic ☐ Cubic

☐ Tetragonal

Crystal (Symmetry Allowed) ▼

☐ Centrosymmetric

☐ Non-centrosymmetric:

☐ Enantiomorphic ☐ Pyro / Piezo (p)

☐ Optical Activity ☐ Piezo (2nd Harm.)

Atomic Environment Type

| Symbol | Elements |
|--------|----------|
| | |

Space Group ▼

Space Group Symbol

Crystal Data

Reduced Cell

Author's Cell

Supercell/Subcell

Axis (Å)

| | | | | | |
|----|-------|-----|----|-------|-----|
| a: | Value | ESD | α: | Value | ESD |
| b: | Value | ESD | β: | Value | ESD |
| c: | Value | ESD | γ: | Value | ESD |

Axial Ratio

| | | |
|------|-------|-----|
| c/a: | Value | ESD |
| a/b: | Value | ESD |
| c/b: | Value | ESD |

Volume

| | |
|-------|-----|
| Value | ESD |
|-------|-----|

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Filters based on the volume of the crystal data.

Filters based on the lengths of the three axes of the crystal data.

Search Window

Reduced Cell

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

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- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Crystal System

- ☐ Tridinic (Anorthic)
- ☐ Rhombohedral
- ☐ Monoclinic
- ☐ Hexagonal
- ☐ Orthorhombic
- ☐ Cubic
- ☐ Tetragonal

Crystal (Symmetry Allowed) ▼

- ☐ Centrosymmetric
- ☐ Non-centrosymmetric:
 - ☐ Enantiomorphic
 - ☐ Pyro / Piezo (p)
 - ☐ Optical Activity
 - ☐ Piezo (2nd Harm.)

Atomic Environment Type

| Symbol | Elements |
|--------|----------|
| | |

Space Group ▼

Space Group Symbol

Crystal Data

Reduced Cell

Author's Cell

Supercell/Subcell

Axis (Å)

| a | b | c |
|-------|-------|-------|
| Value | Value | Value |
| ESD | ESD | ESD |

Volume

| Value |
|-------|
| Value |
| ESD |

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

The reduced cell is a unique, primitive cell based on the three shortest lattice translations.

Filters based on the volume of the reduced cell.

Filters based on the lengths of the three axes of the reduced cell.

Search Window

Author's Cell

Search

Subfile ▼

- Custom PDF Set
 - Alkaloid
 - Amino Acid, Peptide & Complex
 - Battery Material
 - Bioactive
 - No Subclass
 - Depressant
 - Narcotic

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Tridinic (Anorthic) ☐ Rhombohedral ☐ Centrosymmetric ☐

Monoclinic ☐ Hexagonal ☐ Non-centrosymmetric: ☐

Orthorhombic ☐ Cubic ☐ Enantiomorphic ☐ Pyro / Piezo (p) ☐

Tetragonal ☐ Optical Activity ☐ Piezo (2nd Harm.) ☐

Space Group ▼

Space Group Symbol

Crystal Data

Reduced Cell

Author's Cell

Supercell/Subcell

Axis (Å) ▼

a: Value ESD

b: Value ESD

c: Value ESD

α: Value ESD

β: Value ESD

γ: Value ESD

Volume

Value ESD

Molecular/f.u. Volume

Value ESD

Convert Cell

Author's Crystal System: Tridinic (Anorthic) ▼

Author's Lattice Centering: Primitive ▼

Cell Type: Crystal ▼

Convert

Cancel

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Convert Cell form used to convert Author's Cell Axis/Volume data to Crystal or Reduced Cell Axis/Volume data for searching.

Filters based on the lengths of the three axes of the author's cell.

Filters based on the volume of the author's cell.

Search Window

Supercell/Subcell

This search uses derivative lattices (including superlattices and sublattices) generated from the given primary lattices. The volume of superlattices |Q| can be between 1 and 9 and volume of sublattices |X| can be changed from 1/1 to 1/9. Derivative matrices are generated based on the selected volumes. Multiplying derivative matrices by the primary lattices gives derivative lattices, which are then transformed to reduced lattices for searching.

The screenshot shows the ICDD Search Window interface. The left sidebar contains a list of search criteria: Modulated, Diffraction, Physical Properties, Reference, and Comments. A red arrow points to the 'Supercell/Subcell' option under the 'Reference' category. The main window is divided into several sections: 'Subfile' (Custom PDF Set, Alkaloid), 'Environment' (Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data), 'Status' (Primary, Alternate, Deleted), 'Quality Mark' (Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision), 'Database' (ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05)), 'Crystal (Symmetry Allowed)' (Centrosymmetric, Non-centrosymmetric, Enantiomorphic, Pyro / Piezo (p), Optical Activity, Piezo (2nd Harm.)), 'Atomic Environment Type' (Symbol, Elements), 'Space Group' (Space Group Symbol), 'Crystal Data' (Reduced Cell, Author's Cell, Supercell/Subcell), 'Axis (Å)' (a, b, c, Value, ESD), and 'Volume Ratio' (Supercell, Subcell, Volume Ratio: 1 to 1). The 'Supercell/Subcell' option is selected, and the 'Volume Ratio' is set to 1 to 1.

Search Window

Modulated

Search

Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternative
- ☐ Disordered

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Modulated Dimension

- ☐ 3 + 1d
- ☐ 3 + 2d
- ☐ 3 + 3d

Subsystems

- ☐ Modulated Structure (One Subsystem)
- ☐ Composite Structure (Multiple Subsystems)

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Filters based on the number of dimensions used to describe the modulation where "3 + 1d", "3 + 2d", "3 + 3d" indicate one, two, and three additional dimensions respectively.

Filters patterns based on the number of subsystems present in the structure. Composite structures have more than one subsystem.

Search Window

Diffraction

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Radiation: ☒ X-ray/Electron ☐ CW Neutron

Strong Line (Å) ▼

Value ESD

Long Line (Å) ▼

Value ESD

Classifications

☒ D1 ☒ D2 ☒ D3

☒ L1 ☒ L2 ☒ L3

Reported Intensity

☐ Integrated Intensities ☐ Peak Intensities

I/I-corundum ▼

Value ESD

R-factor ▼

Value ESD

Smith-Snyder Figure of Merit ▼

Value ESD

Temperature of Data Collection (K) ▼

Value ESD

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Filters based on the ratio of the intensity of the strongest line of the pattern to the intensity of the strongest line of corundum in a 50/50 weight mixture.

Filters based on the SS/FOM. The figure of merit generally used is that reported by Smith & Snyder, which indicates the completeness & accuracy of measured interplanar spacings.

Search Window

Physical Properties

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Melting Point (K) ▼

Value ESD

Density (g/cm³) ▼

Value ESD

☒ Measured Density ☒ Calculated Density ☒ Structural Density

Color ▼

- Black
- Blue
- Brown
- Color Missing
- Colorless
- Gray
- Green
- Metallic
- Orange
- Pink
- Red

☐ Property Sheet

Search Reset Tab Reset All Help Numeric Input ▼ Global Operator ▼

Filters based on the measured, calculated or structural density of the material.

- Kelvin (K)
- Celsius (°C)
- Fahrenheit (°F)
- Not

Filters based on the melting point. Specify degrees Celsius, Kelvin or Fahrenheit by selecting from the drop down menu.

Search Window

References

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
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 - Narcotic
 - Pesticide & Antimicrobial

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Search All Re

DOI

Title ▼

Author ▼

Publication ▼

Volume ▼

Year

Start Year

End Year

Ambient

Press. (Non-ambient)

Temp. (Non-ambient)

Press. & Temp. (Non-ambient)

Atomic Coordinates

Raw Diffraction Data

Refine your search by selecting filters based upon the journal references of a material.

Select filters by DOI, Title (article title), Author (author name), Journal/Patent, Coden (journal coden), Volume, and Year (publication year).

(05)

Journal/Patent

CODEN

Contains Fragments

Contains Phrase

Exactly

Not

Search

Reset Tab

Reset All

Help

Numeric Input ▼ Global Operator ▼

Search Window

Comments

Search

Subfile ▼

- Custom PDF Set
 - Alkaloid
 - Amino Acid, Peptide & Complex
 - Battery Material
- Bioactive
 - No Subclass
 - Depressant
 - Narcotic
 - Pesticide & Antimicrobial

Environment

- ☐ Ambient
- ☐ Press. (Non-ambient)
- ☐ Temp. (Non-ambient)
- ☐ Press. & Temp. (Non-ambient)
- ☐ Atomic Coordinates
- ☐ Raw Diffraction Data

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

- ☒ Star
- ☒ Good
- ☐ Indexed
- ☐ Calculated
- ☐ Prototyping
- ☐ Minimal Acceptable
- ☐ Blank
- ☐ Low-Precision

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ CSD (02)
- ☐ NIST (03)
- ☐ LPF (04)
- ☐ ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Database Comments ▼

Filter based on the text contained in comments.

Search

Reset Tab

Reset All

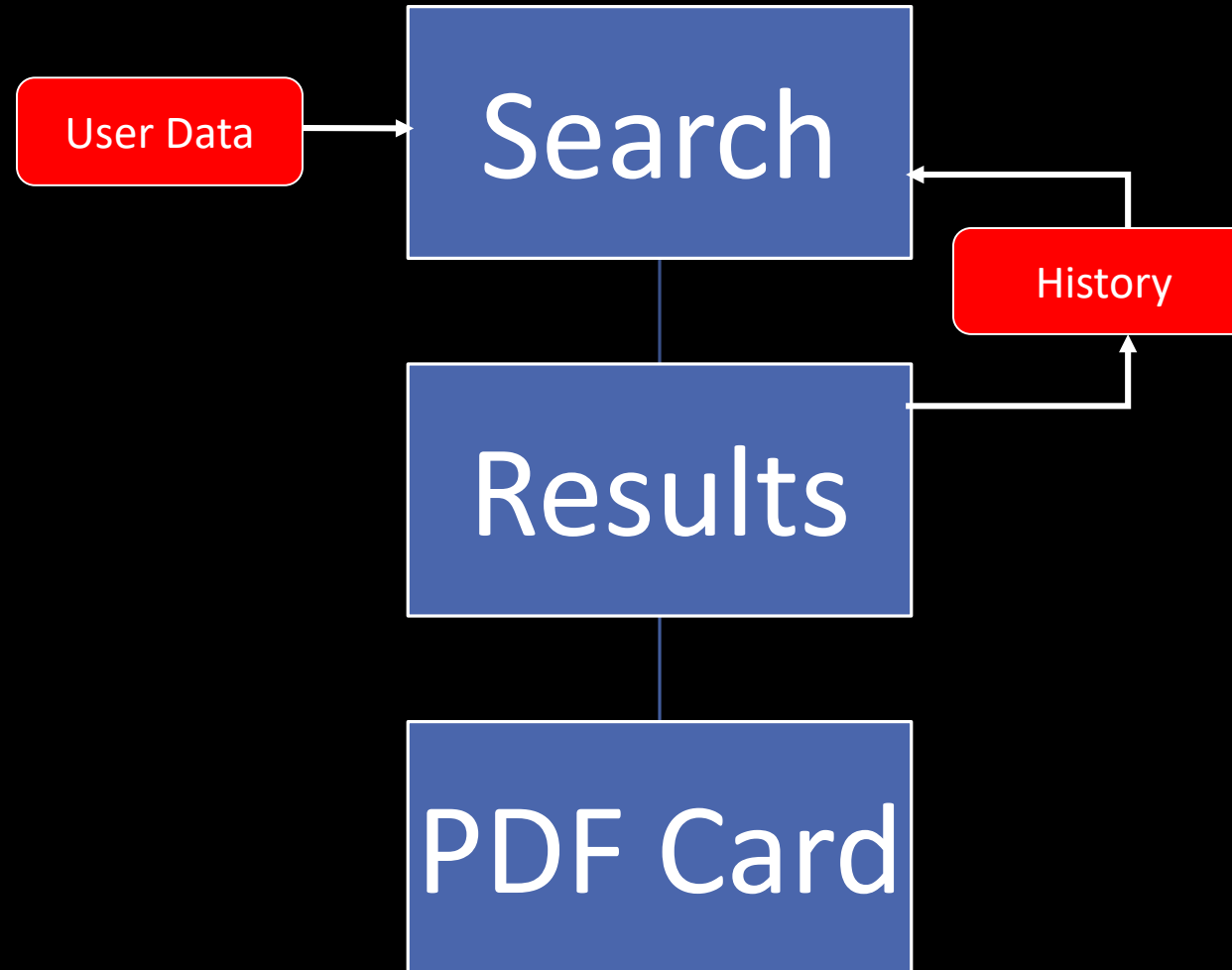
Help

Numeric Input ▼ Global Operator ▼

Data Mining Basics

- Select your filter criteria
- Make use of logical Boolean operators, text and list boxes
- Search
- Review results
- Refine search with additional criteria

Note: Selected search criteria is highlighted in red to keep track of your selections.



Search Example

Select Elements in Periodic Table

The image displays three overlapping screenshots of the ICDD Search software interface, illustrating the search process for Potassium Platinum Chloride. Red annotations highlight key steps:

- Select Elements in Periodic Table:** A red arrow points to the 'H' (Hydrogen) element in the periodic table within the top-left screenshot.
- Select Space Group:** A red arrow points to the 'P4/mmm' space group in the 'Space Group Symbol' dialog box in the bottom-left screenshot.
- Select Compound Name:** A red arrow points to the 'Potassium Platinum Chloride' entry in the 'Name' dropdown menu in the bottom-right screenshot.

The interface includes various search filters such as 'Custom PDF Set', 'Environment', 'Status', 'Quality Mark', 'Database', 'Periodic Table', 'Crystal System', 'Crystallography', 'Modulated', 'Diffraction', 'Physical Properties', 'Reference', and 'Comments'. The bottom-right screenshot shows the search criteria: 'Formula: Any Formula', 'Name: Potassium Platinum Chloride', 'IMA No.', 'CAS Number', 'Number of Elements: Low to High', and 'Composition: Element, Weight %, ESD'.

Selected filters highlighted in red

Search Results

Results - 8 of 298,258

File Fields Set: My Defaults Tools Help

| PDF # | QM | Chemical Formula | Search Results | D1 (Å) | D2 (Å) | D3 (Å) | SYS |
|-------------|----|---|---------------------------------------|----------|----------|----------|-----|
| 00-009-0367 | I | $K_2 Pt Cl_4$ | Potassium Platinum Chloride | 6.940000 | 3.160000 | 3.550000 | T |
| 01-070-1408 | S | $K_2 Pt Cl_4$ | Potassium Platinum Chloride | 7.027500 | 3.182740 | 3.569850 | T |
| 01-073-1506 | I | $K_2 (Pt Cl_4)$ | Potassium Platinum Chloride | 6.990000 | 3.169250 | 3.555730 | T |
| 01-074-1616 | I | $K_2 (Pt (CN)_4) Cl_{0.32} (H_2 O)_{2.6}$ | Potassium Platinum Chloride Cyanid... | 9.866000 | 4.412210 | 6.976320 | T |
| 01-076-2175 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum Chloride | 7.024000 | 3.183270 | 3.571050 | T |
| 01-077-1947 | S | $K_2 Pt Cl_4$ | Potassium Platinum Chloride | 7.023000 | 3.183810 | 3.571940 | T |
| 01-080-0953 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum Chloride | 6.996100 | 3.159080 | 3.540590 | T |
| 01-080-0954 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum Chloride | 6.981300 | 3.156210 | 3.538480 | T |

[(Pt And Cl)] And [Any Name Contains Fragments 'Potassium' And 'Platinum' And 'Chloride'] And [Space Group Symbol Exactly 'P4/mmm'] And [Status (Primary, Alternate)]

Search Filters

Double-click on a PDF number to view the entire PDF Card.



Preferences Module

Open the Preferences Module to select which data fields you would like to display in your results.

You can also select the order in which the data fields are displayed.

Preferences

General Search Diffraction Pattern Sieve

Set ▼ My Defaults ▼

Available Fields

- ICDD Filters
- Formula/Name
- Classifications
- Crystallography
- Diffraction
- Physical Properties
- Reference
- Comments

Selected Fields

- PDF #
- QM
- Chemical Formula
- Compound Name
- D1 (Å)
- D2 (Å)
- D3 (Å)
- SYS

Include Deleted Patterns

OK Cancel Apply Reset Help

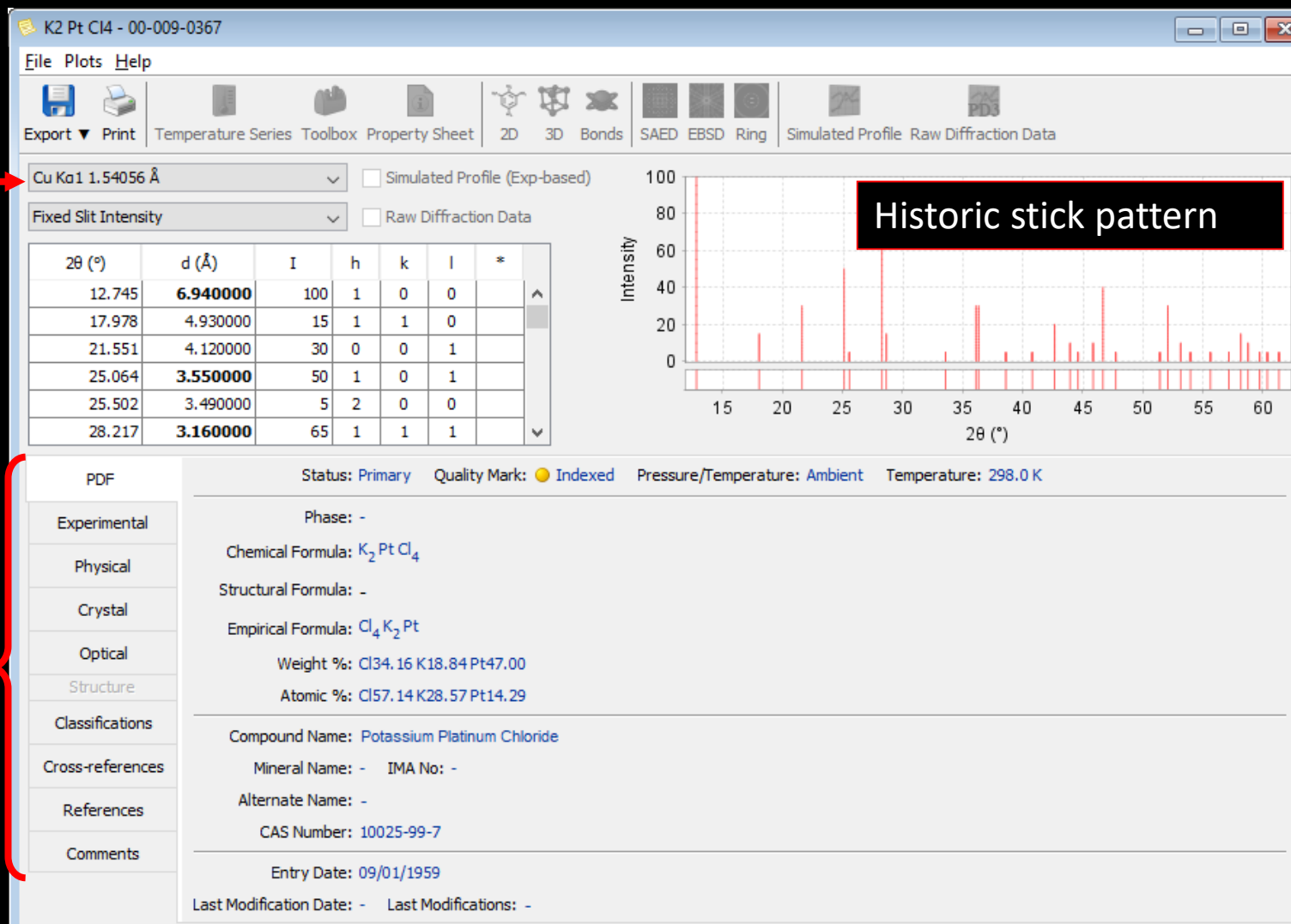
Add data fields to selected list

Order the data fields in the selected list

Remove data fields from the selected list

PDF Data Card

Choose
equipment
factors



Tabular view of reported data

PDF Data Card

Results - 8 of 298,258

File Fields Set: My Defaults Tools Help

| PDF # | QM | Chemical Formula | Compound |
|-------------|----|---|--------------------|
| 00-009-0367 | I | $K_2 Pt Cl_4$ | Potassium Platinum |
| 01-070-1408 | S | $K_2 Pt Cl_4$ | Potassium Platinum |
| 01-073-1506 | I | $K_2 (Pt Cl_4)$ | Potassium Platinum |
| 01-074-1616 | I | $K_2 (Pt (CN)_4) Cl_{0.32} (H_2 O)_{2.6}$ | Potassium Platinum |
| 01-076-2175 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum |
| 01-077-1947 | S | $K_2 Pt Cl_4$ | Potassium Platinum |
| 01-080-0953 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum |
| 01-080-0954 | S | $K_2 (Pt Cl_4)$ | Potassium Platinum |

[[Pt And Cl]] And [Any Name Contains Frag Alternate]]

Open PDF Card

Add to Custom PDF Set...

Remove from Custom PDF Set...

Tools/Simulations

Copy PDF #

Select All

Remove Rows

Open multiple PDF Cards.

Hold the Ctrl key, then select PDF cards. Right click mouse, select Open PDF Card.

K2 Pt Cl4 - 00-009-0367

File Plots Help

Export Print

K2 Pt Cl4 - 01-070-1408

File Plots Help

Export Print

K2 (Pt Cl4) - 01-076-2175

File Plots Help

Export Print

Temperature Series Toolbox Property Sheet 2D 3D Bonds SAED EBSD Ring Simulated Profile Raw Diffraction Data

Cu Kα1 1.54056 Å

Fixed Slit Intensity

Simulated Profile (Calc)

Raw Diffraction Data

| 2θ (°) | d (Å) | I | h | k | l | * |
|--------|-----------------|-----|---|---|---|---|
| 12.592 | 7.024000 | 999 | 1 | 0 | 0 | |
| 17.844 | 4.966720 | 102 | 1 | 1 | 0 | |
| 21.409 | 4.147000 | 230 | 0 | 0 | 1 | |
| 24.913 | 3.571050 | 390 | 1 | 0 | 1 | |
| 25.339 | 3.512000 | 65 | 2 | 0 | 0 | |
| 28.007 | 3.183270 | 521 | 1 | 1 | 1 | |

Intensity

2θ (°)

Status: Alternate Quality Mark: Star Pressure/Temperature: Ambient Temperature: 298.0 K

Phase: -

Chemical Formula: $K_2 (Pt Cl_4)$

Structural Formula: -

Empirical Formula: $Cl_4 K_2 Pt$

Weight %: Cl34.16 K18.84 Pt47.00

Atomic %: Cl57.14 K28.57 Pt14.29

Compound Name: Potassium Platinum Chloride

Mineral Name: - IMA No: -

Alternate Name: potassium tetrachloroplatinate(II)

CAS Number: -

Entry Date: 09/01/1998

Last Modification Date: 09/01/2016 Last Modifications: Quality



Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD® website.
www.icdd.com

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