

# 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.

The screenshot shows the PDF-2 2018 software interface. At the top is a menu bar with 'File', 'Edit', 'Window', and 'Help'. Below it is a toolbar with icons for 'Open PDF Cards', 'Preferences', 'Search History', 'Results', and 'Sieve Microanalysis'. A red box highlights this toolbar, with a red arrow pointing to a label 'Tool Bar' on the left. Below the toolbar is a 'Search' window with several filter sections: 'Subfile' (a tree view showing categories like 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', etc.), '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', 'Deleted'), 'Quality Mark' (radio buttons for 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', 'Minimal Acceptable', 'Blank', 'Low-Precision'), and 'Database' (checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', 'ICDD Crystal Data (05)'). Below these filters is a 'Periodic Table' with columns labeled IA through VIIIA. The table contains element symbols, atomic numbers, and names. A search bar is positioned above the table with options for 'Boolean Search' and 'Yes/No/Maybe Search', and a 'Set Unselected to No' button. At the bottom of the search window are buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help', along with a 'Numeric Input' and 'Global Operator' dropdown.

Tool Bar

Primary Search Menu

# Getting Started

The screenshot shows the PDF-2 software interface. The 'File' menu is open, and the 'Enter PDF Numbers' dialog box is displayed. The 'File' menu item is circled in red, with a red arrow pointing to the 'Open PDF Cards...' option. The 'Enter PDF Numbers' dialog box has a red box around the 'Enter PDF Numbers' title bar with an arrow pointing to the 'PDF Number' input field. Another red box is around the 'Recent PDF Cards' dropdown menu with an arrow pointing to the list of recent PDF cards.

**File** Edit Window Help

Open PDF Cards Preferences Search History Results Sieve+ Microanalysis

Open PDF Cards... Ctrl+O

Close All PDF Cards

New Diffraction Pattern

Print User Comments...

Restore Settings

Exit

Enter PDF Numbers

PDF Number: - -

Recent PDF Cards

Na ( N O3 ) - 01-089-0310

S - 00-001-0478

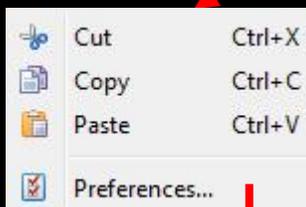
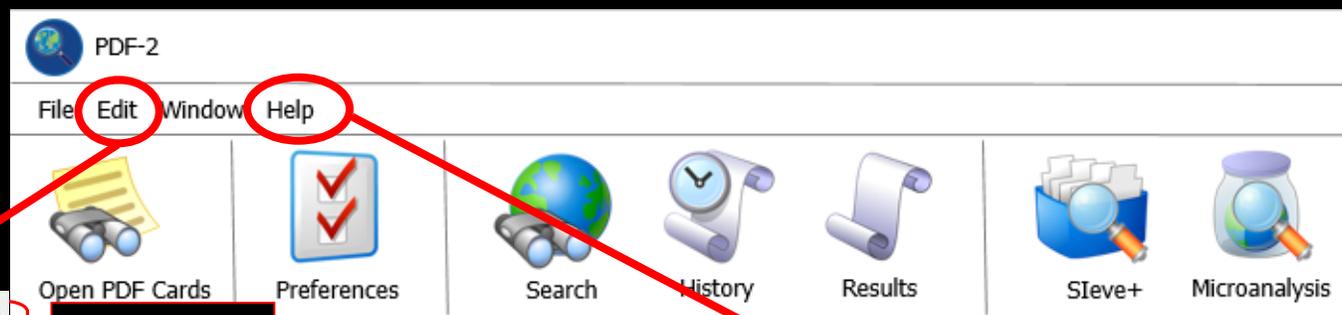
C9 H8 N Na O3 - 00-001-0002

Open Clear Cancel

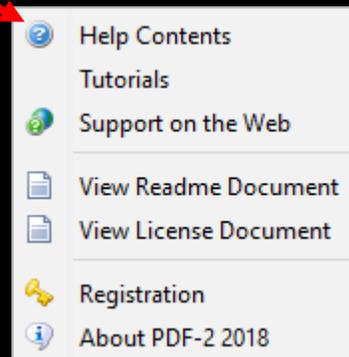
Open a known PDF card.

Navigate quickly to a recent PDF card.

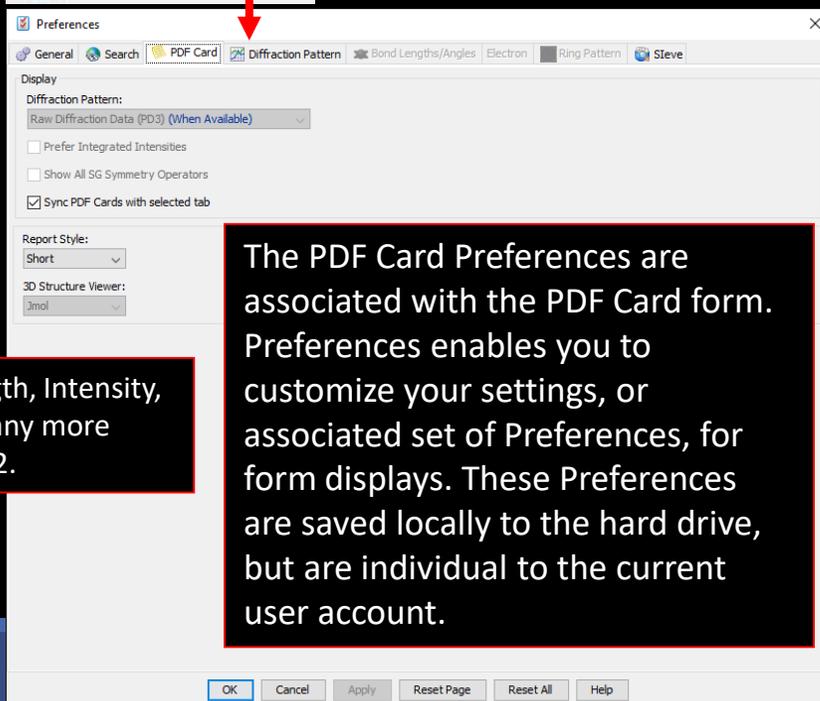
# Getting Started



Edit functions



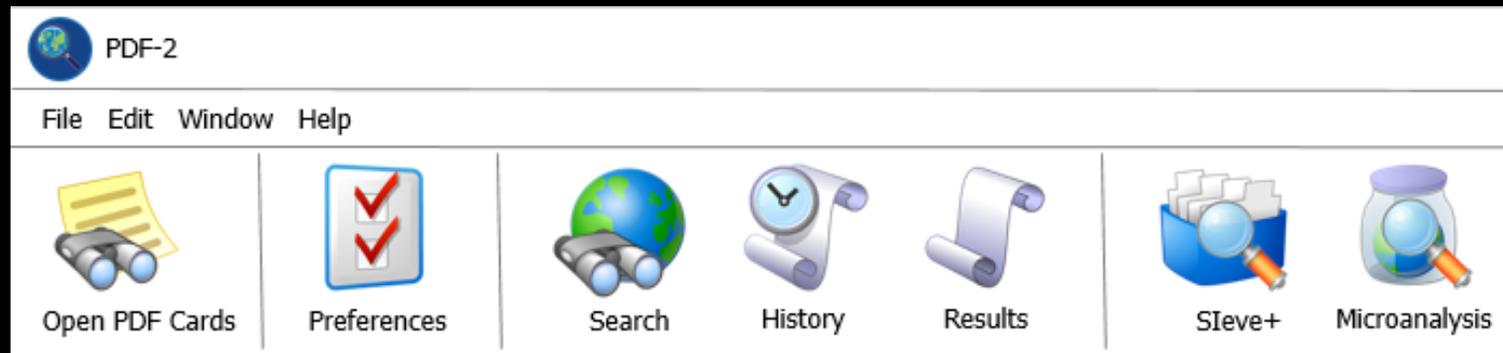
Help information regarding use, support, license policy, and registration of the PDF-2. Be sure to register the PDF-2 by clicking on Registration within 10 days of installation to activate the full license term.



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 shows the ICDD Primary Search Menu interface. The window is titled "Search" and contains several panels 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)", and "Press. & Temp. (Non-ambient)".
- Status:** Checkboxes for "Primary", "Alternate", and "Deleted".
- Quality Mark:** A legend with color-coded circles for "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)".

Below these panels is a periodic table with search criteria applied to elements. The search criteria are indicated by colored boxes on the periodic table and a search bar at the bottom. The search bar contains the text "Search" and "Reset Tab", "Reset All", "Help" buttons. The search criteria are: "Boolean Search" (selected), "Yes/No/Maybe Search", "And", "Or", "Not", "Grouping:", "Only", "Just", "And", "Or".

# Search Window

## Subfiles/Database Filters

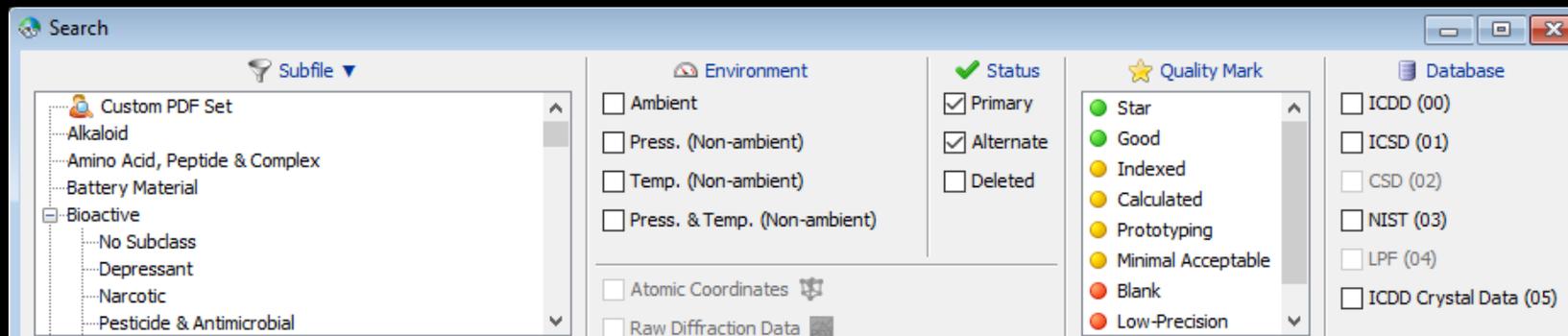
The screenshot displays the 'Search' window with the following sections:

- 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 levels: 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)'.
- Search Options:** Radio buttons for 'Boolean Search' (selected) and 'Yes/No/Maybe Search'. Includes 'And', 'Or', 'Not', 'Only', and 'Just' options, along with 'Grouping' controls.
- Periodic Table:** A standard periodic table with elements highlighted in various colors (green, yellow, red, blue, cyan) corresponding to the search filters.
- Bottom Panel:** Includes a 'Search' button, 'Reset Tab', 'Reset All', 'Help', and a 'Numeric Input' field with a 'Global Operator' dropdown.

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

# 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 shows the ICDD Search Window interface. On the left, there is a 'Subfile' dropdown menu with a tree view containing categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. Below this is a 'Periodic Table' section with a grid of elements. Each element cell contains its symbol, atomic number, and atomic weight. The elements are color-coded by group: IA (green), IIA (cyan), IIIA (blue), IVB (purple), VB (orange), VIB (red), VIIB (pink), VIIIB (light blue), IB (yellow), IIB (light green), IIIA (light blue), IVA (purple), VA (orange), VIA (red), VIIA (pink).

On the right side of the search window, there are several filter sections:
 

- Environment:** Includes checkboxes for 'Ambient', 'Press. (Non-ambient)', 'Temp. (Non-ambient)', 'Press. & Temp. (Non-ambient)', 'Atomic Coordinates', and 'Raw Diffraction Data'.
- Status:** Includes checkboxes for 'Primary' (checked), 'Alternate' (checked), and 'Deleted'.
- Quality Mark:** Includes a list of quality marks with corresponding colored circles: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (orange), and Low-Precision (orange).
- ICDD:** Includes checkboxes for 'ICDD', 'ICSD', 'CSD', 'NIST', 'LPF', and 'ICDD'.

In the center, there is a search input field with a dropdown menu showing 'Boolean Search' (selected) and 'Yes/No/Maybe Search'. Below the input field are radio buttons for 'And', 'Or', and 'Not', and a 'Grouping:' section with 'And' and 'Or' radio buttons. A red arrow points to the 'Boolean Search' dropdown.

At the bottom, there is a 'Search' button, 'Reset Tab', 'Reset All', and 'Help' buttons. There is also a 'Numeric Input' and 'Global Operator' dropdown menu.

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

The screenshot shows a software interface for searching through a database. It features several filter panels at the top: 'Subfile' (with a tree view of categories like 'Custom PDF Set', 'Alkaloid', etc.), 'Environment' (with checkboxes for 'Ambient', 'Press. (Non-ambient)', etc.), 'Status' (with checkboxes for 'Primary', 'Alternate', 'Deleted'), 'Quality Mark' (with radio buttons for 'Star', 'Good', 'Indexed', etc.), and 'Database' (with checkboxes for 'ICDD (00)', 'ICSD (01)', etc.).

Below the filters is a 'Periodic Table' section. It includes a grid of element symbols and atomic weights, color-coded by search status. A search bar above the table has radio buttons for 'Boolean Search' and 'Yes/No/Maybe Search', with a red arrow pointing to the latter. A 'Set Unselected to No' button is also present.

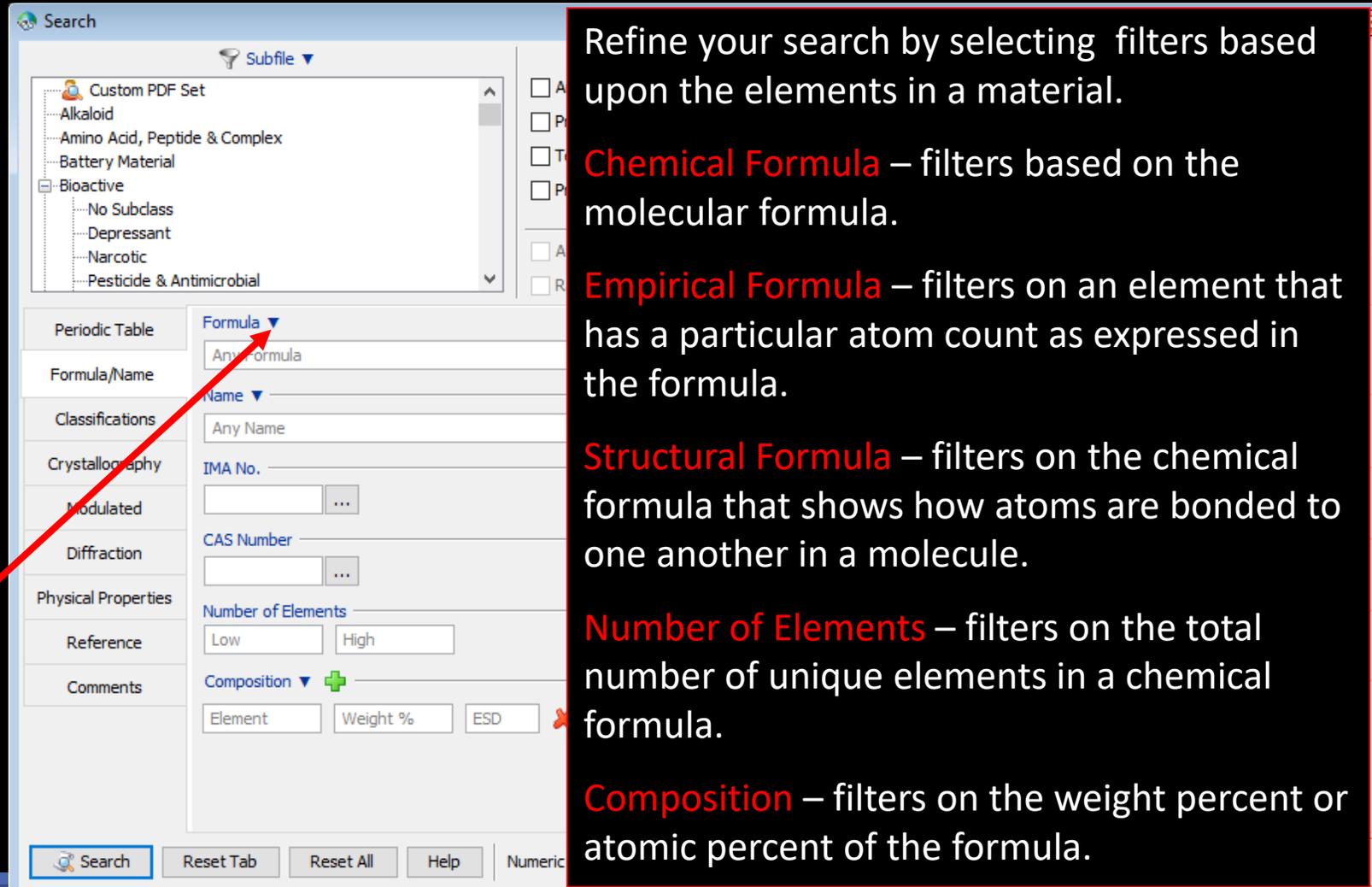
At the bottom of the window are buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help', along with a 'Numeric Input' field and a 'Global Operator' dropdown.

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



The screenshot shows a search interface with a tree view on the left containing categories like 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The main search area has several filter sections: 'Periodic Table', 'Formula/Name', 'Classifications', 'Crystallography', 'Modulated', 'Diffraction', 'Physical Properties', 'Reference', and 'Comments'. The 'Formula/Name' section is expanded, showing a dropdown menu with options: 'Any Formula', 'Chemical Formula', 'Empirical Formula', 'Structural Formula', 'Contains Elements', 'Contains Phrase', 'Exactly', and 'Not'. A red arrow points from the 'Formula' dropdown in the main interface to the 'Any Formula' option in the expanded menu. Below the search area are buttons for 'Search', 'Reset Tab', 'Reset All', 'Help', and '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 a software interface for searching materials. It features several filter panels: 'Subfile' with a tree view of categories like 'Alkaloid' and 'Bioactive'; 'Environment' with checkboxes for 'Ambient', 'Press. (Non-ambient)', etc.; 'Status' with checkboxes for 'Primary', 'Alternate', and 'Deleted'; 'Quality Mark' with a list of quality levels like 'Star', 'Good', 'Indexed', etc.; and 'Database' with checkboxes for 'ICDD (00)', 'ICSD (01)', etc. Below these is a search section with a 'Formula' dropdown set to 'Any Formula' and a 'Name' dropdown set to 'Any Name'. A red arrow points from the 'Name' dropdown to a callout box. The bottom of the window has a 'Search' button and 'Reset Tab', 'Reset All', and 'Help' buttons.

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

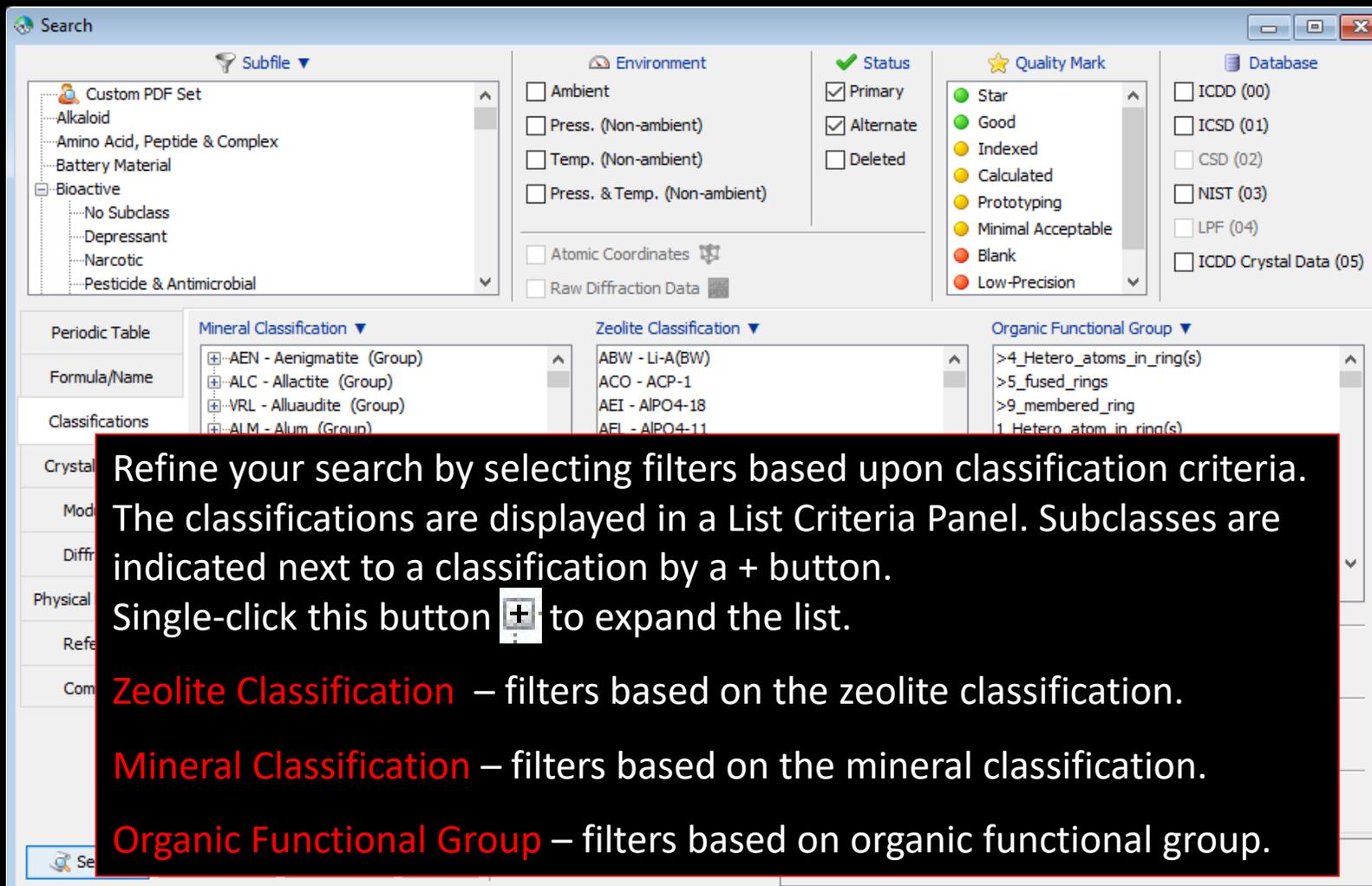
**Compound Name** – filters based on the compound name.

**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 'Search' window with several filter panels:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (expanded to show 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).
- Classification Panels:**
  - Mineral Classification:** AEN - Aenigmatite (Group), ALC - Allactite (Group), VRL - Alluaudite (Group), ALM - Alum. (Group).
  - Zeolite Classification:** ABW - Li-A(BW), ACO - ACP-1, AEI - AlPO4-18, AFI - AlPO4-11.
  - Organic Functional Group:** >4\_Hetero\_atoms\_in\_ring(s), >5\_fused\_rings, >9\_membered\_ring, 1\_Hetero\_atom\_in\_ring(s).

**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. At the top, there are tabs for Subfile, Environment, Status, Quality Mark, and Database. The Environment tab is active, showing checkboxes for Ambient, Press. (Non-ambient), Temp. (Non-ambient), and Press. & Temp. (Non-ambient). The Status tab shows checkboxes for Primary, Alternate, and Deleted. The Quality Mark tab shows a list of quality marks: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision. The Database tab shows checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05).

Below these tabs, there are several classification and filter sections:

- 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 - Ancylite (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.

At the bottom, there are filter sections for Pearson Symbol, Prototype Structure, and Formula Type (ANX). The Pearson Symbol filter is set to "With Hydrogen". The Prototype Structure filter is set to "Any Prototype Structure".

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

Filters for Pearson Symbol Codes with and without Hydrogen.

Filters based on a user-constructed Pearson Symbol Code.

# Search Window Crystallography

Search Window Crystallography interface showing various search filters and options. The Crystallography tab is highlighted, displaying additional search tabs: *Crystal Data*, *Reduced Cell*, *Author's Cell*, and *Supercell/Subcell*.

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 Window

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)
- Monoclinic
- Orthorhombic
- Tetragonal
- Rhombohedral
- Hexagonal
- Cubic

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

Volume

Value

ESD

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 Window

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)

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)

Axis	Value	ESD
a:	Value	ESD
b:	Value	ESD
c:	Value	ESD

Reduced Cell

Author's Cell

Supercell/Subcell

Axial Ratio

Ratio	Value	ESD
a/b:	Value	ESD
b/c:	Value	ESD
c/a:	Value	ESD

Volume

Volume	Value	ESD
Volume	Value	ESD

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

Filters based on the volume of the crystal data.

Search

Reset Tab

Reset All

Help

Numeric Input

Global Operator

# Search Window

## Reduced Cell

The screenshot shows the 'Search' window with various filters and options. The 'Crystal System' section includes checkboxes for Tridinic (Anorthic), Rhombohedral, Monoclinic, Hexagonal, Orthorhombic, Cubic, and Tetragonal. The 'Crystal (Symmetry Allowed)' section includes checkboxes for Centrosymmetric, Non-centrosymmetric, Enantiomorphic, Pyro / Piezo (p), Optical Activity, and Piezo (2nd Harm.). The 'Atomic Environment Type' section includes Symbol and Elements. The 'Space Group' section includes a Space Group Symbol field. The 'Crystal Data' section includes Reduced Cell, Author's Cell, and Supercell/Subcell. The 'Axis (Å)' section includes fields for a, b, and c, each with a Value and ESD field. The 'Volume' section includes a Value and ESD field.

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

The screenshot shows the 'Search' window with several filter panels: 'Subfile', 'Environment', 'Status', 'Quality Mark', and 'Database'. The 'Author's Cell' section is expanded, showing options for 'Crystal Data', 'Reduced Cell', 'Author's Cell', and 'Supercell/Subcell'. The 'Author's Cell' section includes input fields for 'a', 'b', and 'c' axes, 'Volume', and 'Molecular/f.u. Volume'. A 'Convert Cell' dialog box is open, showing 'Author's Crystal System' set to 'Tridinic (Anorthic)', 'Author's Lattice Centering' set to 'Primitive', and 'Cell Type' set to 'Crystal'. The dialog has 'Convert' and 'Cancel' buttons.

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 volume of the author's cell.

Filters based on the lengths of the three axes 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 'Search' window with the following 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** (highlighted with a red arrow)
- Axis (Å):** a, b, c;  $\alpha$ ,  $\beta$ ,  $\gamma$
- Volume Ratio:** 1 to 1
- Supercell/Subcell:** Radio buttons for Supercell (selected) and Subcell

Buttons at the bottom: Search, Reset Tab, Reset All, Help, Numeric Input, Global Operator

# Search Window Modulated

Search

Subfile

Environment

Status

Quality Mark

Database

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

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

Environment

Status

Quality Mark

Database

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

Melting Point (K)

Value

ESD

Density (g/cm<sup>3</sup>)

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

Environment

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

DOI

Title

Author

Publication

Volume

Year

Start Year

End Year

Search All Re

Search

Reset Tab

Reset All

Help

Numeric Input

Global Operator

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).

- Journal/Patent
- CODEN
- Contains Fragments
- Contains Phrase
- Exactly
- Not

# Search Window

## Comments

The screenshot shows a 'Search' window with several filter panels:

- Subfile:** A tree view showing categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive' (with sub-items: 'No Subclass', 'Depressant', 'Narcotic', 'Pesticide & Antimicrobial'), 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 with colored circles: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (red), and Low-Precision (red).
- Database:** Checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'.

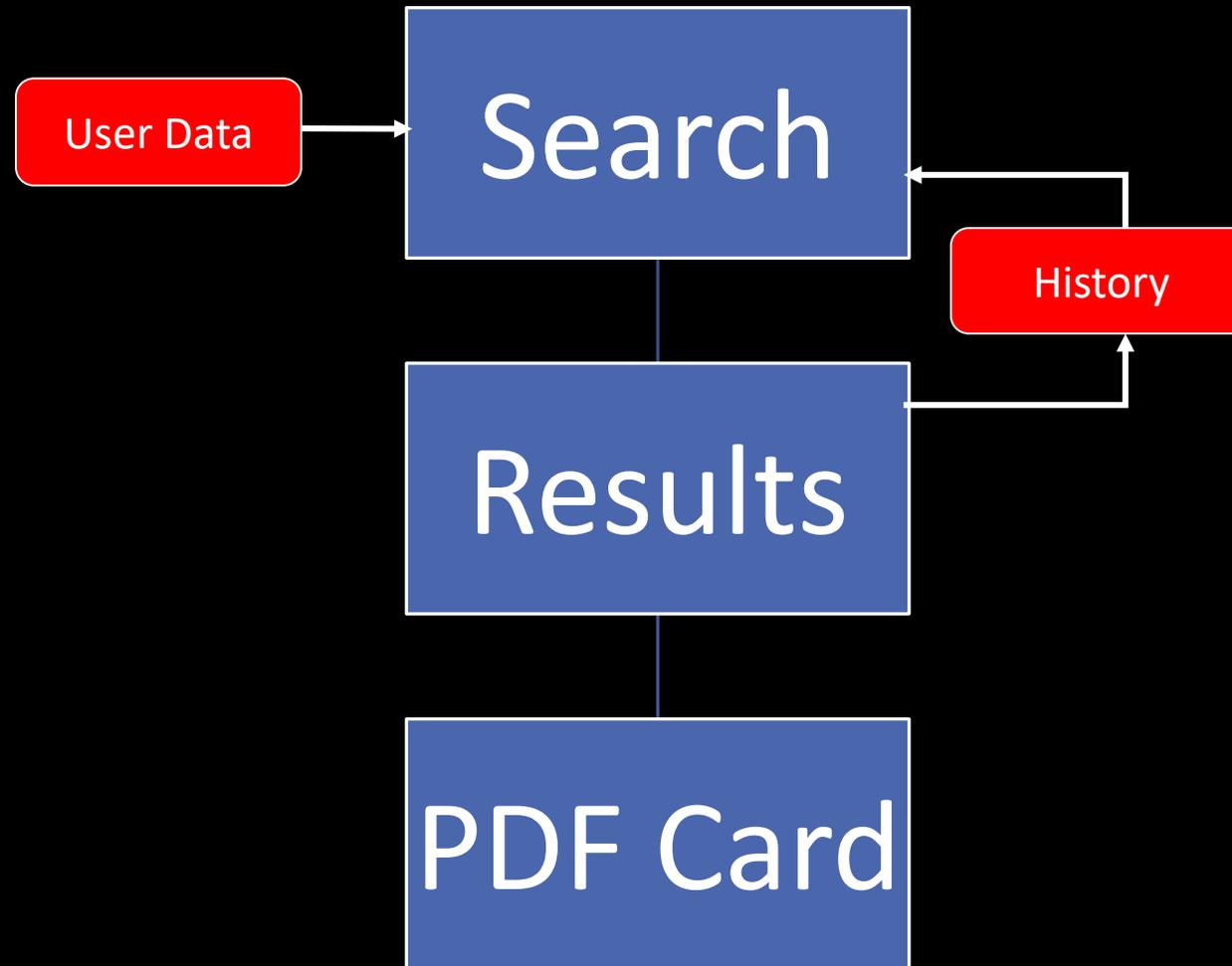
Below the filters is a 'Database Comments' section with a search input field and a list of comment categories:

- Absolute Configuration
- Additional Diffraction Lines
- Additional Patterns
- Analysis
- ANX
- Atomic Position
- Bioactivity
- Boiling Point
- Calculated Pattern Original Remarks

A red-bordered box highlights the search input field with the text: "Filter based on the text contained in comments."

At the bottom of the window are buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help', along with dropdown menus for 'Numeric Input' and '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

Select Space Group

Select Compound Name

Selected filters highlighted in red

# Search Results

Results - 8 of 298,258

File Fields Set: My Defaults Tools Help

PDF #	QM	Chemical Formula	Name	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 Results

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.

The screenshot shows the 'Preferences' dialog box with the 'Search' tab selected. The 'Set' dropdown is set to 'My Defaults'. The 'Available Fields' list on the left includes folders for ICDD Filters, Formula/Name, Classifications, Crystallography, Diffraction, Physical Properties, Reference, and Comments. The 'Selected Fields' list on the right contains PDF #, QM, Chemical Formula, Compound Name, D1 (Å), D2 (Å), D3 (Å), and SYS. A right-pointing arrow button is positioned between the two lists, and a left-pointing arrow button is below it. At the bottom, there is an 'Include Deleted Patterns' checkbox and buttons for 'OK', 'Cancel', 'Apply', 'Reset', and '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

The screenshot shows the ICDD software interface for a PDF Data Card. The window title is "K2 Pt Cl4 - 00-009-0367". The menu bar includes "File", "Plots", and "Help". The toolbar contains icons for "Export", "Print", "Temperature Series", "Toolbox", "Property Sheet", "2D", "3D", "Bonds", "SAED", "EBSD", "Ring", "Simulated Profile", and "Raw Diffraction Data".

Below the toolbar, there are two dropdown menus: "Cu Ka1 1.54056 Å" and "Fixed Slit Intensity". To the right of these are two checkboxes: "Simulated Profile (Exp-based)" and "Raw Diffraction Data".

A table displays diffraction data:

2θ (°)	d (Å)	I	h	k	l	*
12.745	<b>6.940000</b>	100	1	0	0	
17.978	4.930000	15	1	1	0	
21.551	4.120000	30	0	0	1	
25.064	<b>3.550000</b>	50	1	0	1	
25.502	3.490000	5	2	0	0	
28.217	<b>3.160000</b>	65	1	1	1	

To the right of the table is a plot of Intensity vs 2θ (°). The plot shows a series of peaks, with the most prominent ones at 12.745°, 25.064°, and 28.217°. A red box highlights the plot with the text "Historic stick pattern".

Below the table and plot is a section for the PDF Data Card. It includes a sidebar with tabs for "PDF", "Experimental", "Physical", "Crystal", "Optical", "Structure", "Classifications", "Cross-references", "References", and "Comments". The main area displays the following information:

- Status: Primary
- Quality Mark: Indexed
- Pressure/Temperature: Ambient
- Temperature: 298.0 K
- Phase: -
- Chemical Formula:  $K_2PtCl_4$
- Structural Formula: -
- Empirical Formula:  $Cl_4K_2Pt$
- 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: -
- CAS Number: 10025-99-7
- Entry Date: 09/01/1959
- Last Modification Date: - Last Modifications: -

Historic stick pattern

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 Chloride
01-070-1408	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride
01-073-1506	I	$K_2 (Pt Cl_4)$	Potassium Platinum Chloride
01-074-1616	I	$K_2 (Pt (CN)_4) Cl_{0.32} (H_2 O)_{2.6}$	Potassium Platinum Chloride
01-076-2175	S	$K_2 (Pt Cl_4)$	Potassium Platinum Chloride
01-077-1947	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride
01-080-0953	S	$K_2 (Pt Cl_4)$	Potassium Platinum Chloride
01-080-0954	S	$K_2 (Pt Cl_4)$	Potassium Platinum Chloride

[[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

K2 Pt Cl4 - 01-070-1408

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 Ka1 1.54056 Å

Fixed Slit Intensity

Simulated Profile (Calc)

Raw Diffraction Data

2θ (°)	d (Å)	I	h	k	l	*
12.592	<b>7.024000</b>	999	1	0	0	
17.844	4.966720	102	1	1	0	
21.409	4.147000	230	0	0	1	
24.913	<b>3.571050</b>	390	1	0	1	
25.339	3.512000	65	2	0	0	
28.007	<b>3.183270</b>	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](http://www.icdd.com)

International Centre for Diffraction Data®  
12 Campus Boulevard  
Newtown Square, PA 19073  
Phone: 610.325.9814  
Toll Free Number in US & Canada: 866.378.0331  
Fax: 610.325.9823