

# PDF-2 Tools and Searches



# PDF-2 2019

The PDF-2 2019 database is powered by our integrated search display software. PDF-2 2019 boasts 69 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 2019.

PDF-2 2019

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
  - Psychotropic
  - Stimulant

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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

Search

Reset Tab

Reset All

Help

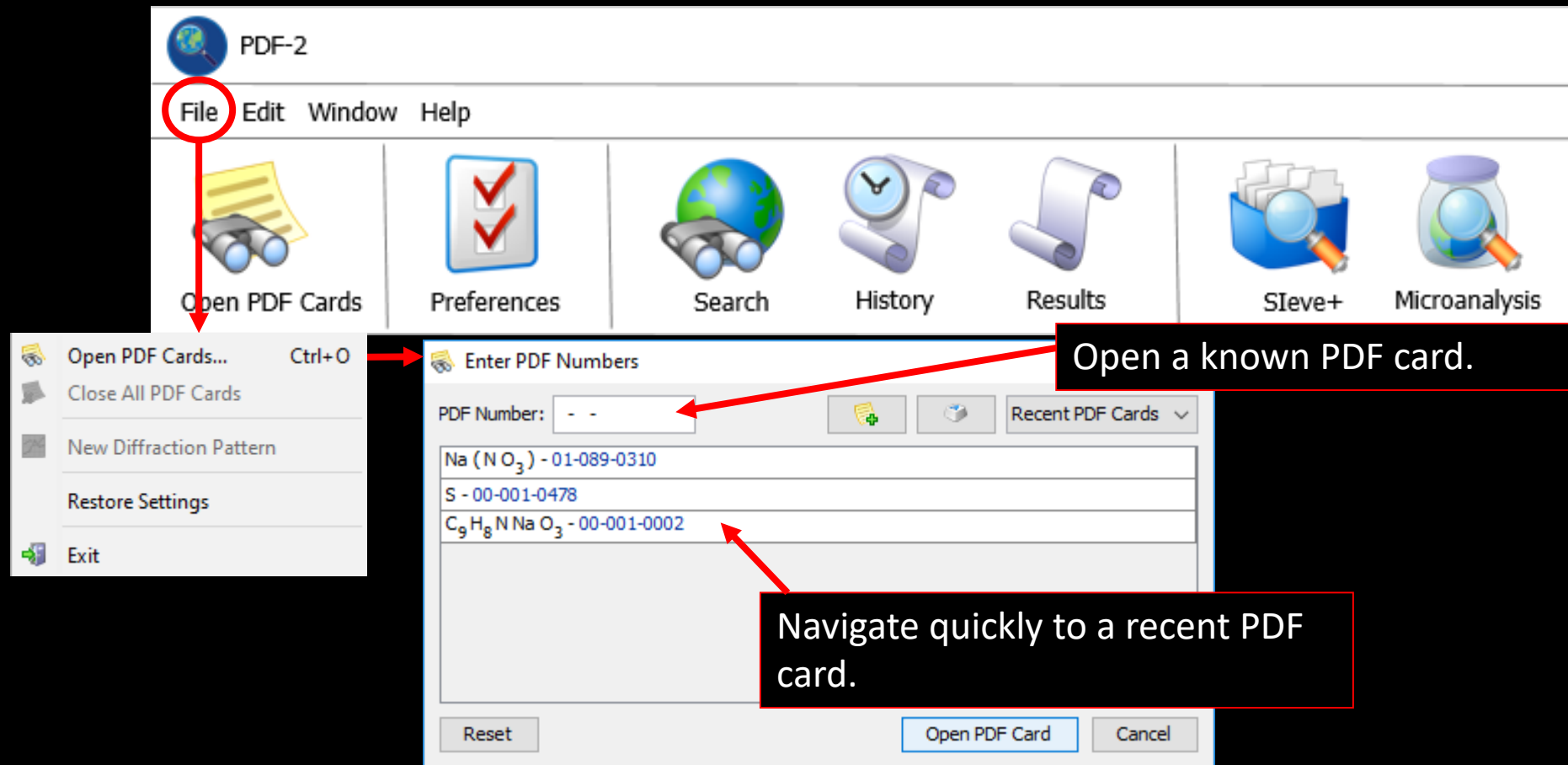
Range Input

Global Operator

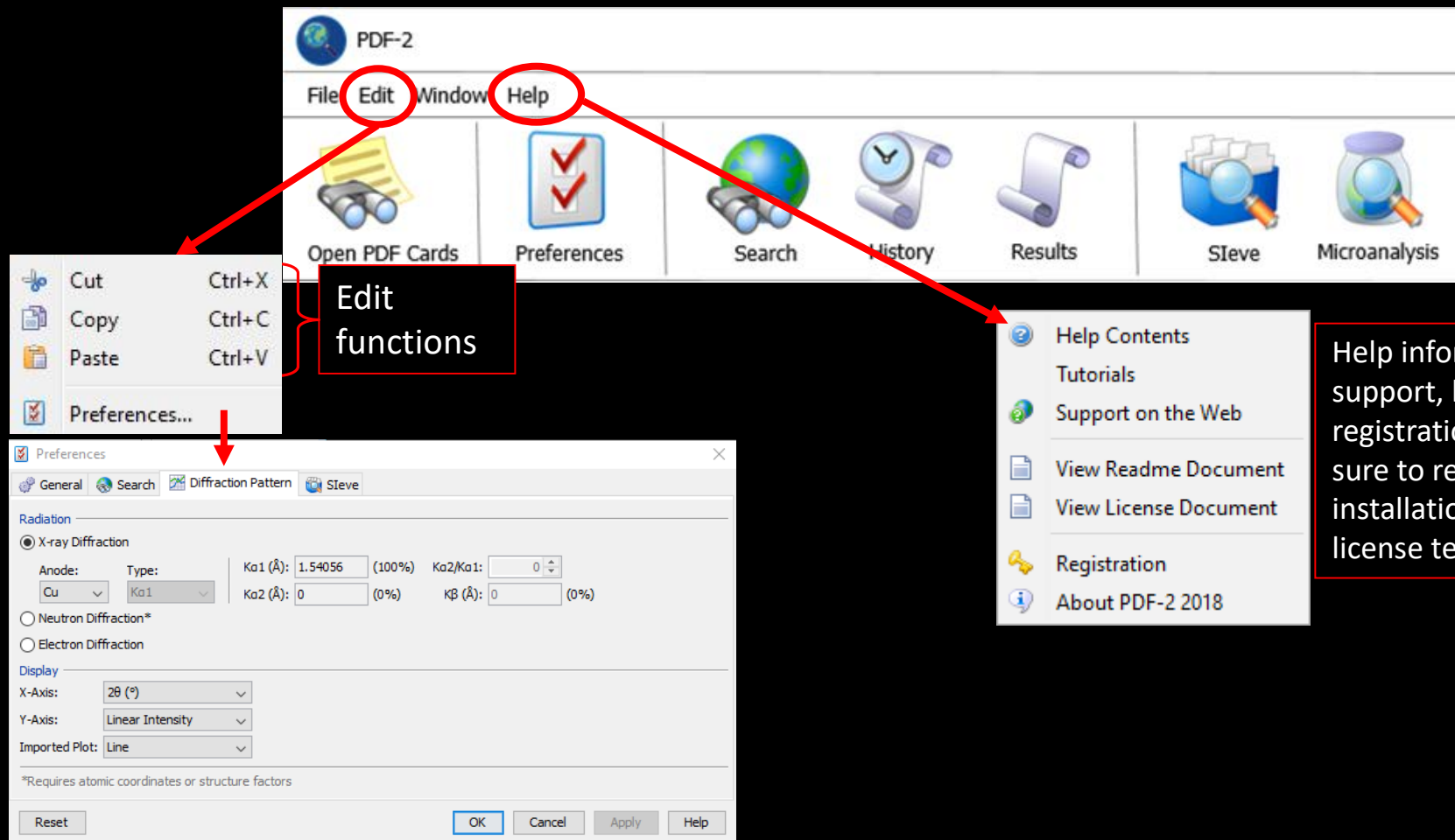
Tool Bar

Primary Search Menu

# Getting Started



# Getting Started



The screenshot shows the PDF-2 software interface. The main menu bar includes File, Edit, Window, and Help. Below the menu bar are icons for Open PDF Cards, Preferences, Search, History, Results, SIeve, and Microanalysis. The Edit menu is open, showing options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), and Preferences... The Help menu is also open, showing options: Help Contents, Tutorials, Support on the Web, View Readme Document, View License Document, Registration, and About PDF-2 2018. A red box highlights the Edit functions, and another red box highlights the Help information.

**Edit functions**

- Cut (Ctrl+X)
- Copy (Ctrl+C)
- Paste (Ctrl+V)
- Preferences...

**Help information regarding use, support, license policy, and registration of the PDF-2. Be sure to register the PDF-2 upon installation to activate the full license term.**

- Help Contents
- Tutorials
- Support on the Web
- View Readme Document
- View License Document
- Registration
- About PDF-2 2018

**Preferences**

General Search Diffraction Pattern SIieve

**Radiation**

☒ X-ray Diffraction

Anode: Cu Type: Ka1 Ka1 (Å): 1.54056 (100%) Ka2/Ka1: 0 Ka2 (Å): 0 (0%) Kβ (Å): 0 (0%)

☐ Neutron Diffraction\*

☐ Electron Diffraction

**Display**

X-Axis: 2θ (°)

Y-Axis: Linear Intensity

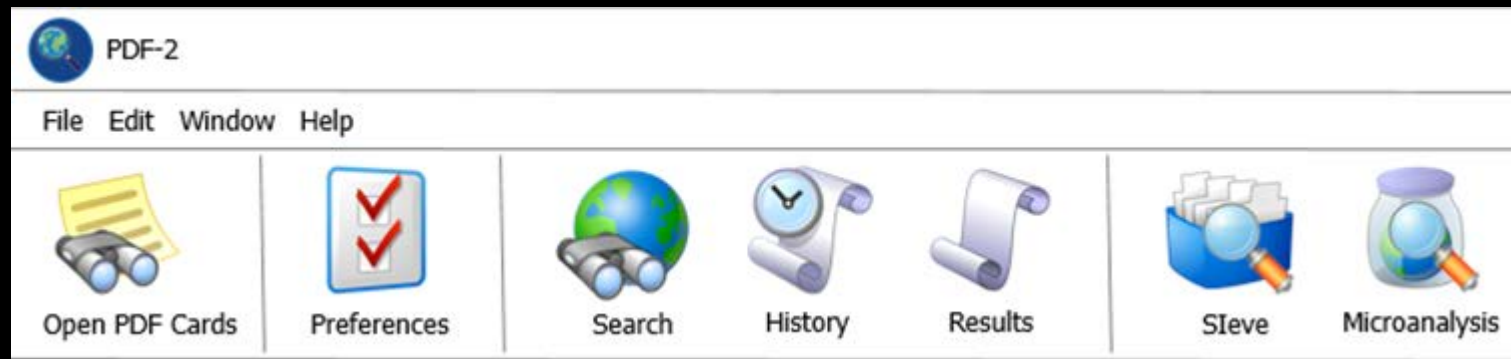
Imported Plot: Line

\*Requires atomic coordinates or structure factors

Reset OK Cancel Apply Help

Customize Radiation, Display settings, 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 'Search' window of the ICDD software. The interface is divided into several sections:

- Subfile:** A tree view on the left showing a hierarchy of categories: Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (with sub-items: No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, Stimulant), and others.
- Environment:** Checkboxes for Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, and Raw Diffraction Data.
- Status:** Checkboxes for Primary (checked), Alternate, and Deleted.
- Quality Mark:** A list of quality levels with corresponding colored circles: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (orange), Low-Precision (red), and Hypothetical (red).
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05).
- Periodic Table:** A central periodic table with elements color-coded by group. To its left are tabs for Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. To its right are search logic options: Boolean (selected), Yes/No/Maybe, and Composition Diagram List, along with And/Or/Not/Just/Only/Just grouping options.
- Search Bar:** At the bottom, there is a 'Search' button, 'Reset Tab', 'Reset All', and 'Help' buttons, followed by a 'Range Input' dropdown and a 'Global Operator' dropdown.

# Search Window

## Subfiles/Database Filters

Search

Subfile ▼

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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 ☒ Yes/No/Maybe ☐ Composition Diagram List

And ☐ Or ☐ Not

Only ☐ Just

Grouping: ☐ And ☐ Or

Search

Reset Tab

Reset All

Help

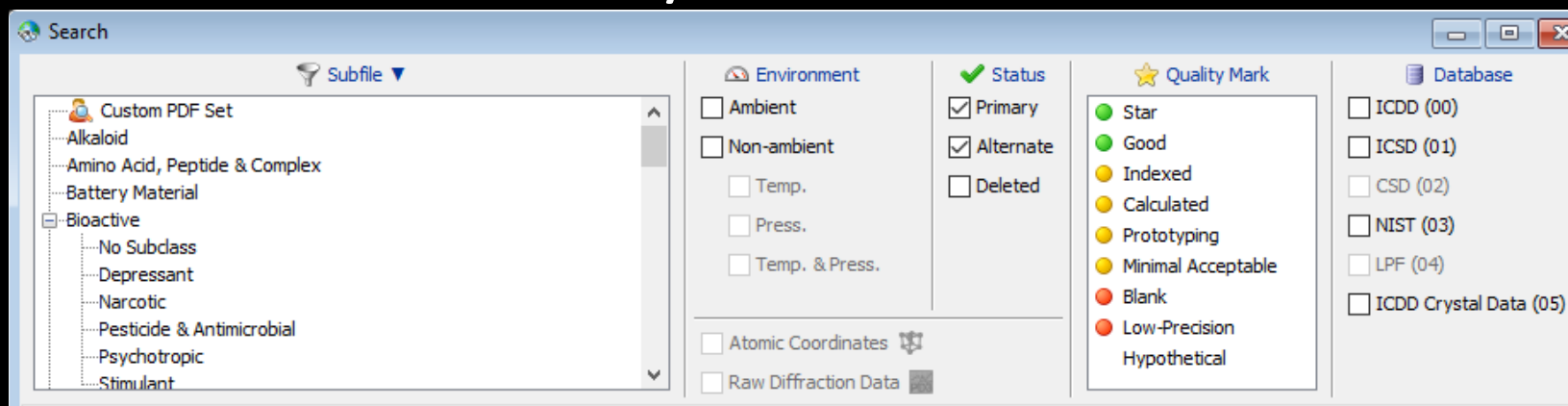
Range Input ▼ Global Operator ▼

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 displays the 'Search' window with several filter sections:

- Subfile:** A tree view under 'Custom PDF Set' including Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (with sub-items: No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, Stimulant), and others.
- Environment:** Checkboxes for Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, and Raw Diffraction Data.
- Status:** Checkboxes for Primary, Alternate, and Deleted.
- Quality Mark:** Radio buttons for Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, and Hypothetical.
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data.

Below the filters is the **Periodic Table** with columns 1 through 18. To the left of the table are search criteria: Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. Between the filter sections and the periodic table is a search logic area with radio buttons for Boolean, Yes/No/Maybe, and Composition Diagram List. Under Boolean, there are options for And, Or, Not, Only, and Just. A red arrow points to the 'Boolean' radio button. Below these are 'Grouping' and 'Composition Diagram List' buttons.

At the bottom of the window are buttons for Search, Reset Tab, Reset All, Help, Range Input, and Global Operator.

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

Search Window Interface showing filters and the periodic table.

**Filters:**

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, Stimulant.
- Environment:** Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary, Alternate, Deleted.
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, Hypothetical.
- 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.

Search, Reset Tab, Reset All, Help, Range Input, Global Operator.

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

## Periodic Table Filters

**Composition Diagram List** - This lists all phases in a binary system (if two elements are selected), all phases in a ternary system (if three elements are selected), and all phases in a quaternary system (if four elements are selected). The phases are sorted by atomic fraction (using the empirical formula), going from one side of the phase diagram to the other side.

Select one or more phases from the list and click Search to view all of the PDF entries that have the selected empirical formula(s).

The screenshot shows the 'Search' window with the 'Periodic Table Filters' section. The 'Composition Diagram List' radio button is selected. The periodic table is displayed with elements color-coded by quality mark. A list of empirical formulas and hits is shown on the right.

Empirical Formula	Hits
Cl <sub>2</sub>	7
Cl <sub>4</sub> Pt	3
Cl <sub>3</sub> Pt	1
Cl <sub>2</sub> Pt	9
Pt	52

# 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
  - Psychotropic
  - Stimulant

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 % ± Error ✕

Search Reset Tab Reset All Help Range Input

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

Search

Subfile ▼

Custom PDF Set

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

Periodic Table

Formula/Name

Formula ▼

Any Formula

Name ▼

Any Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

IMA No.

CAS Number

Number of Elements

Low High

Composition ▼

Element Weight %

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Search

Reset Tab

Reset All

Help

Range Input ▼ Global Operator ▼

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

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

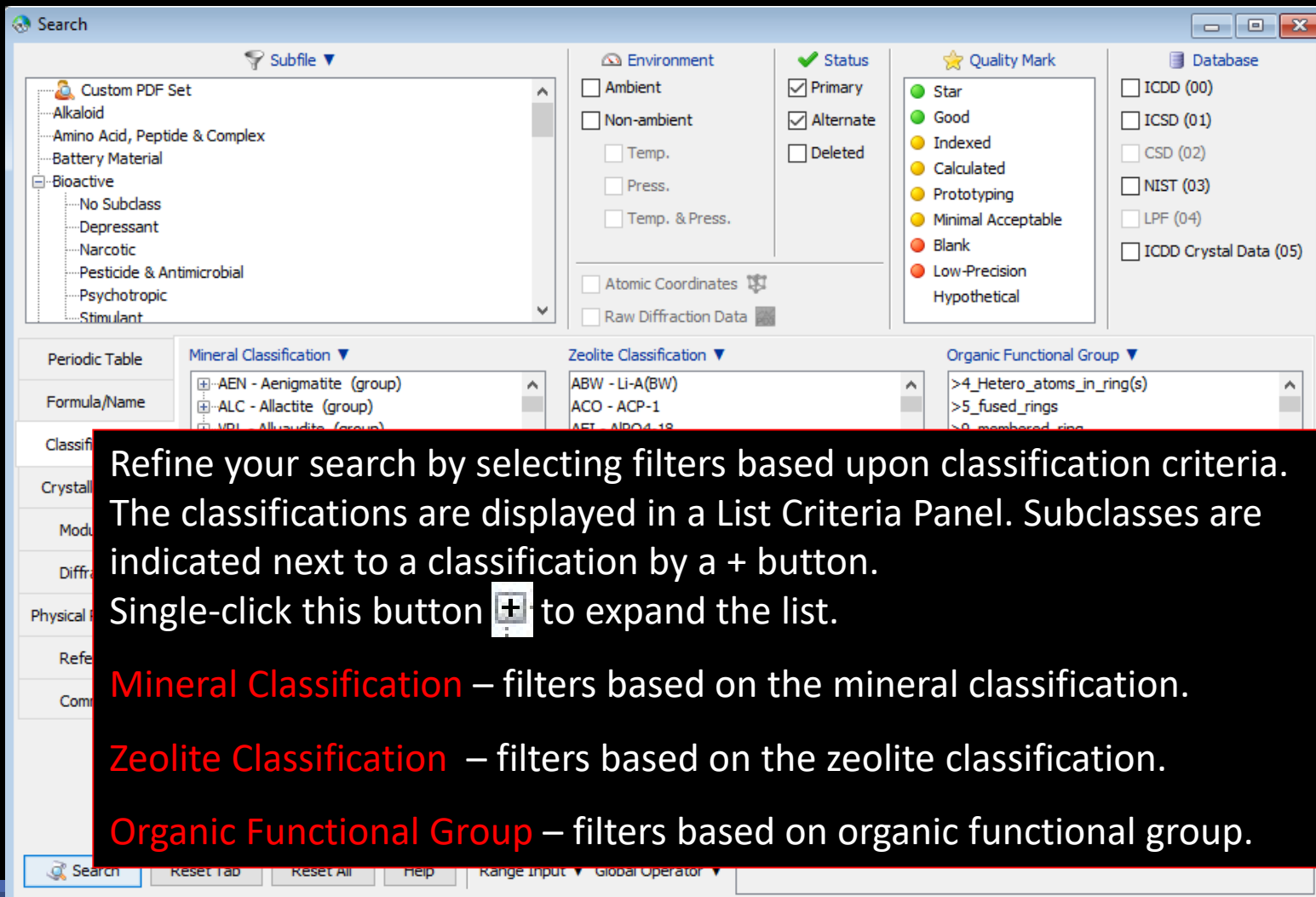
**Mineral Name** – filters based on the mineral name.

**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 of the ICDD database. It features a 'Subfile' dropdown menu, a 'Custom PDF Set' list, and several filter panels. The 'Environment' panel includes checkboxes for 'Ambient', 'Non-ambient', 'Temp.', 'Press.', 'Temp. & Press.', 'Atomic Coordinates', and 'Raw Diffraction Data'. The 'Status' panel has checkboxes for 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' panel shows a list of quality levels with corresponding colored circles: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (red), Low-Precision (red), and Hypothetical (red). The 'Database' panel includes checkboxes for '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, and VPL - Alluvudite), 'Zeolite Classification' (listing ABW - Li-A(BW), ACO - ACP-1, and AET - APO4-18), and 'Organic Functional Group' (listing >4\_Hetero\_atoms\_in\_ring(s), >5\_fused\_rings, and >9\_membered\_ring). A red box highlights the 'Mineral Classification' panel and the 'Organic Functional Group' panel, with 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.

**Mineral Classification** – filters based on the mineral classification.

**Zeolite Classification** – filters based on the zeolite classification.

**Organic Functional Group** – filters based on organic functional group.



# Search Window

## Pearson Symbol Code

The screenshot shows the ICDD Search Window interface. On the left is a sidebar with a tree view under 'Custom PDF Set' containing categories like Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, and Stimulant. Below this is a vertical menu with options: Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The main area is divided into several filter sections: 'Subfile' (a dropdown), 'Environment' (checkboxes for Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data), 'Status' (checkboxes for Primary, Alternate, Deleted), 'Quality Mark' (radio buttons for Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, Hypothetical), and 'Database' (checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05)). Below these are three classification lists: 'Mineral Classification' (AEN - Aenigmatite, ALC - Allactite, VRL - Alluaudite, ALM - Alum, ALN - Alunite, AMB - Amblygonite, AMP - Amphibole, ANC - Analcime, ANY - Ancyrite, ADA - Andalusite, ANT - Antlerite), 'Zeolite Classification' (ABW - Li-A(BW), ACO - ACP-1, AEI - AIPO4-18, AEL - AIPO4-11, AEN - AIPO-EN3, AET - AIPO4-8, AFG - Afghanite, AFI - AIPO4-5, AFN - AIPO-14, AFO - AIPO4-41, AFR - SAPO-40), and 'Organic Functional Group' (>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), 3\_membered\_rinq). At the bottom are input fields for 'Pearson Symbol' (set to 'With Hydrogen'), 'Prototype Structure' (set to 'Any Prototype Structure'), and 'Formula Type (ANX)'. A search bar is at the very bottom with 'Search', 'Reset Tab', 'Reset All', 'Help', 'Range Input', and 'Global Operator' buttons.

Filters for Pearson Symbol Codes with and without Hydrogen.

Filters based on a user-constructed Pearson Symbol Code.



# Search Window

## Crystallography

Search Window

Subfile ▼

Custom PDF Set

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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

Crystal Data

Reduced Cell

Author's Unit Cell

Supercell/Subcell

Axis (Å)

a	b	c
Value ± Error	Value ± Error	Value ± Error

Axial Ratio

c/a	a/b
Value ± Error	Value ± Error

Volume

Value	± Error

Search

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
  - Psychotropic
  - Stimulant

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Property

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

Volume

Value

± Error

Range Input ▼ Global Operator ▼

Search

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
  - Psychotropic
  - Stimulant

Environment

☐ Ambient

☐ Non-ambient

☐ Temp.

☐ Press.

☐ Temp. & Press.

☐ Atomic Coordinates

☐ Raw Diffraction Data

Status

☒ Primary

☒ Alternate

☐ Deleted

Quality Mark

- Star
- Good
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- Prototyping
- Minimal Acceptable
- Blank
- Low-Precision
- Hypothetical

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

Reduced Cell

Author's Unit Cell

Supercell/Subcell

Axis (Å)

a: Value ± Error

b: Value ± Error

c: Value ± Error

α: Value ± Error

β: Value ± Error

γ: Value ± Error

Axial Ratio

c/a: Value ± Error

a/b: Value ± Error

c/b: Value ± Error

Volume

Value ± Error

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

Range Input ▼ Global Operator ▼

# Search Window

## Reduced Cell

Search

Subfile ▼

Custom PDF Set

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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
- ☐ Monodinic
- ☐ 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 Unit Cell

Supercell/Subcell

Axis (Å)

a: Value ± Error

b: Value ± Error

c: Value ± Error

Volume

Value ± Error

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

Filters based on the volume of the reduced cell.

Search

Reset Tab

Reset All

Help

Range 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 Unit Cell

Search

Subfile ▼

Custom PDF Set

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

Environment

- ☐ Ambient
- ☐ Non-ambient
  - ☐ Temp.
  - ☐ Press.
  - ☐ Temp. & Press.

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Convert Cell

Author's Crystal System: Triclinic (Anorthic) ▼

Author's Lattice Centering: Primitive ▼

Cell Type: Crystal ▼

Convert Cancel

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

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

Space Group

Space Group Symbol

Crystal Data

Reduced Cell

Author's Unit Cell

Supercell/Subcell

Axis (Å) ▼

a: Value ± Error

b: Value ± Error

c: Value ± Error

α: Value ± Error

β: Value ± Error

γ: Value ± Error

Axial Ratio

c/a: Value ± Error

a/b: Value ± Error

c/b: Value ± Error

Volume

Value ± Error

Molecular/f.u. Volume

Value ± Error

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

Convert Cell form used to convert Author's Unit 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 unit cell.

Filters based on the volume of the author's unit 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. A red arrow points from the text box on the left to the 'Supercell/Subcell' option in the 'Crystal Data' section. The interface includes various search filters and options:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide, & Complex
- Environment:** Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data
- Status:** Primary, Alternate, Deleted
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, Hypothetical
- 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 Unit Cell, Supercell/Subcell
- Search Parameters:** Axis (A), a: Value ± Error, α: Value ± Error, b: Value ± Error, β: Value ± Error, c: Value ± Error, γ: Value ± Error
- Volume Ratio:** 1 to 1
- Search Type:** Supercell, Subcell

Buttons at the bottom include Search, Reset Tab, Reset All, Help, Range Input, and Global Operator.

# Search Window

## Modulated

Search

Subfile ▼

Custom PDF Set

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐

Quality Mark

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

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ 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

Range 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
  - Psychotropic
  - Stimulant

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

- ☒ D1 ☒ D2 ☒ D3

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Radiation: ☒ X-ray/Electron ☐ CW Neutron

Strong Line (Å) ▼

Value  ± Error

Long Line (Å) ▼

Value  ± Error

Reported Intensity

- ☐ Integrated Intensities ☐ Peak Intensities

I/I-corundum ▼

Value  ± Error

R-factor ▼

Value  ± Error

Smith-Snyder Figure of Merit ▼

Value  ± Error

Temperature of Data Collection (K) ▼

Value  ± Error

Pressure of Data Collection (GPa) ▼

Value  ± Error

Search Reset Tab Reset All Help Range 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
  - Psychotropic
  - Stimulant

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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  ± Error

Density (g/cm³) ▼

Value  ± Error

☒ Measured Density ☒ Calculated Density ☒ Structural Density

Color ▼

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

☐ Property Sheet

☐ Topology Data

Search Reset Tab Reset All Help Range 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

The screenshot shows the 'Search' window in the ICDD software. The 'References' tab is selected in the left sidebar. The 'Publication' field is highlighted with a red arrow, and its dropdown menu is open, showing options: 'Journal/Patent', 'CODEN', 'Contains Fragments', 'Contains Phrase', 'Exactly', and 'Not'. The 'Journal/Patent' option is selected. The 'Search' button is at the bottom left, and the 'Reset All' button is at the bottom center.

Search

Subfile ▼

Custom PDF Set

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

DOI

Title ▼

Author ▼

Publication ▼

Volume ▼

Year

Start Year

End Year

Search All

Search

Reset Tab

Reset All

Help

Range 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

Search

Subfile ▼

Custom PDF Set

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

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.

Absolute Configuration

Additional Diffraction Lines

Additional Patterns

Analysis

ANX

Atomic Position

Bioactivity

Boiling Point

Calculated Pattern Original Remarks

Search

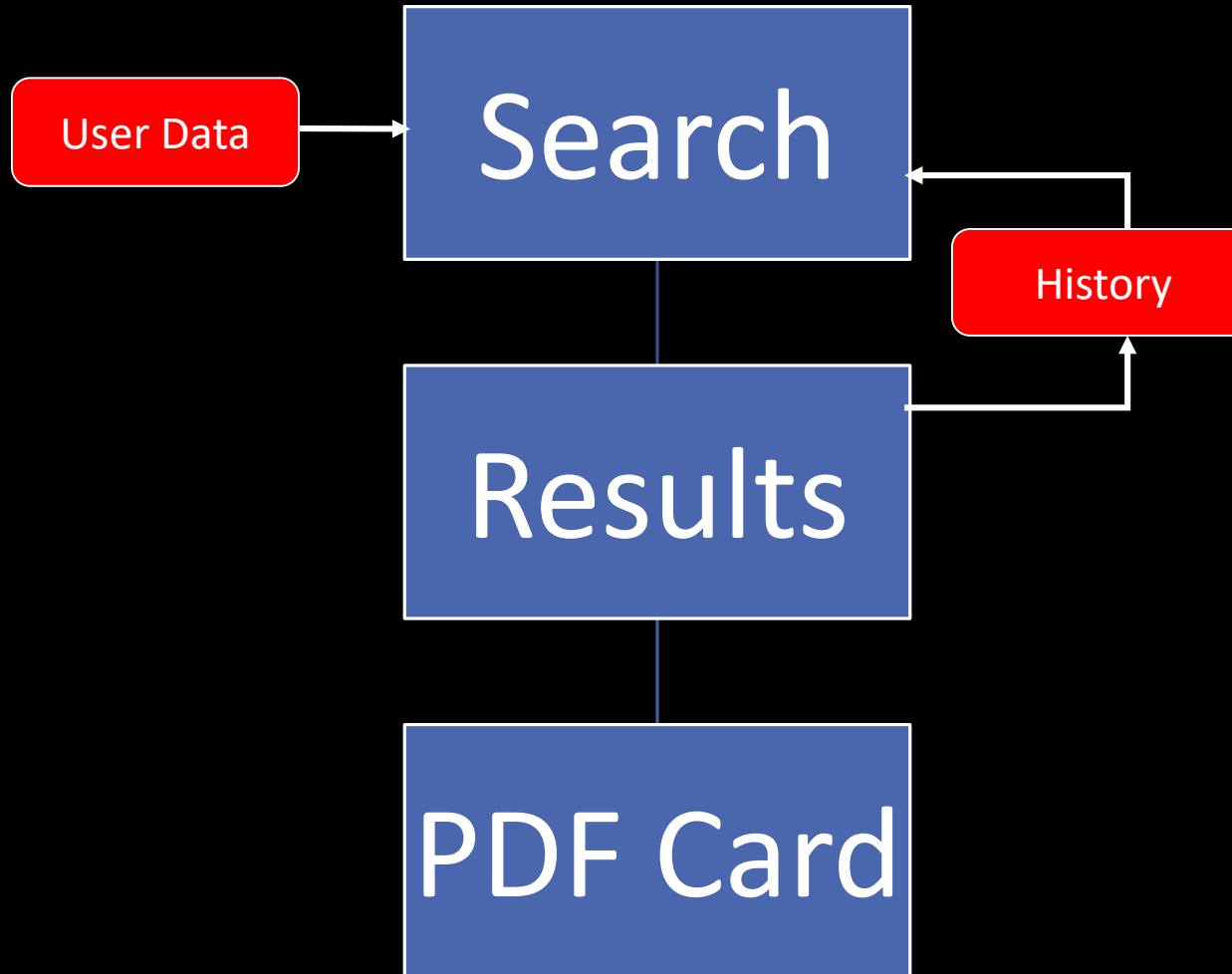
Reset Tab

Reset All

Help

Range 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 screenshot displays the ICDD search interface with three overlapping windows. The top window shows the periodic table with elements H, Li, Be, Na, and Mg highlighted in red. The bottom-left window shows the 'Space Group' dropdown menu with 'P4/mmm' selected. The bottom-right window shows the 'Name' dropdown menu with 'Potassium Platinum Chloride' selected. Red arrows point from the text labels to the corresponding UI elements.

**Select Space Group**

**Select Compound Name**

**Selected filters highlighted in red**

# Search Results

Results - 8 of 304,114

File Fields Tools Help

Open PDF Card Simulated Profile My Defaults

PDF #	QM	Chemical Formula		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 Contains Phrase 'P4/mmm'] And [Status (Primary, Alternate)]

Search Results

Search Filters

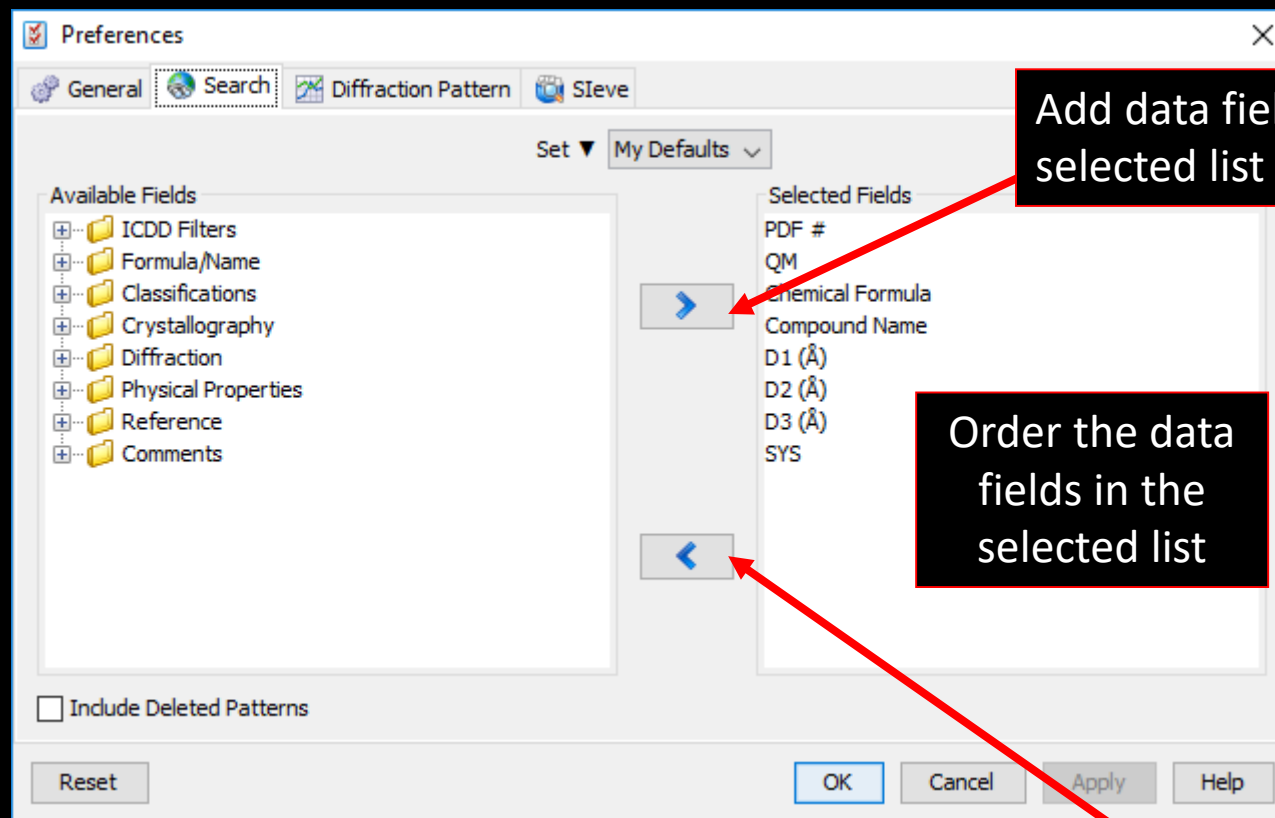
Double-click on a PDF number to view the entire PDF Card.



# 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.



Add data fields to selected list

Order the data fields in the selected list

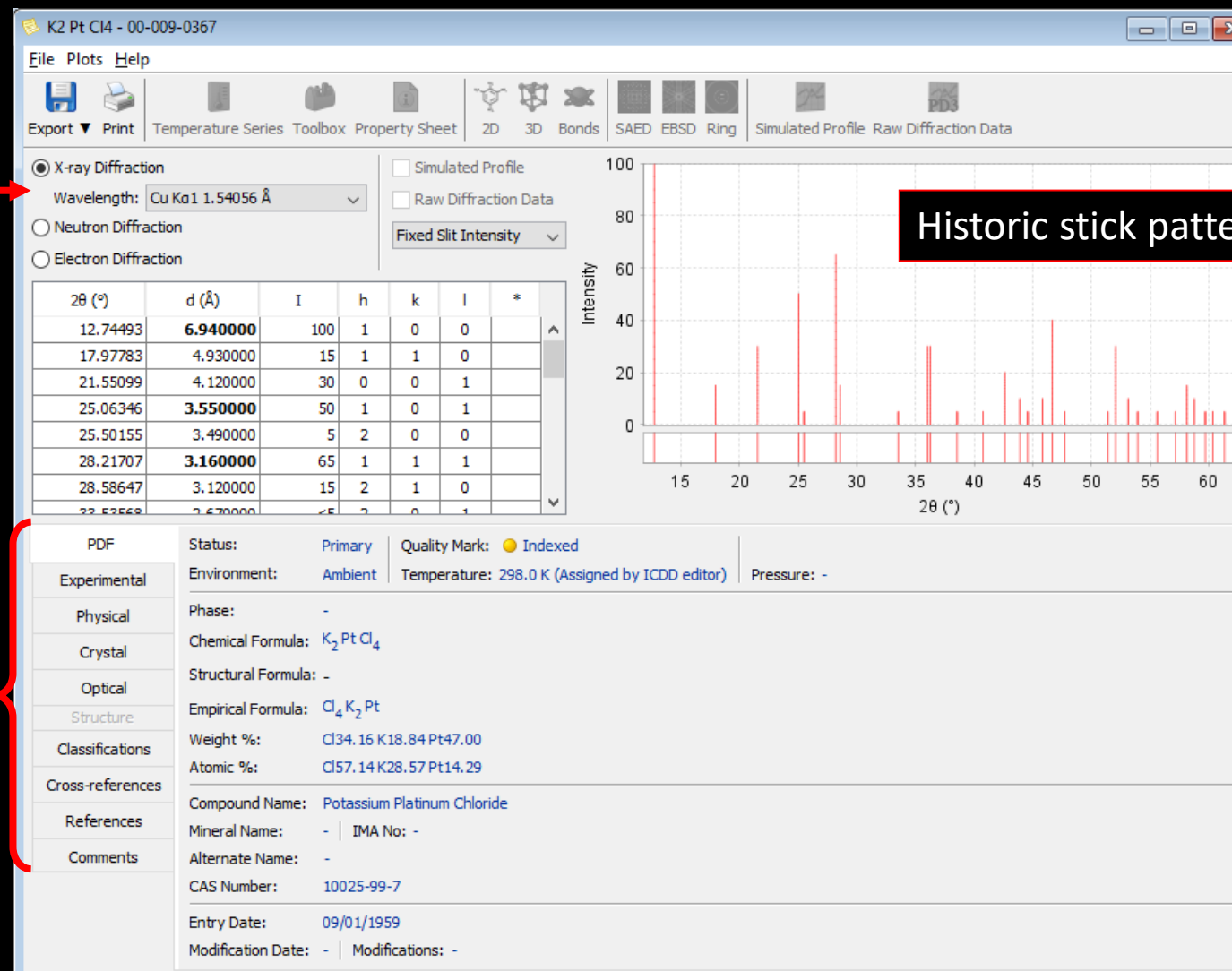
Remove data fields from the selected list

# PDF Data Card

Choose equipment factors

Historic stick pattern

Tabular view of reported data





# PDF Data Card

Results - 8 of 304,114

File Fields Tools Help

Open PDF Card Simulated Profile

PDF #	QM	Chemical Formula	Compound Name
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 Fra (Primary, Alternate)]

Open PDF Card

Add to Custom PDF Set...

Remove from Custom PDF Set...

Tools/Simulations

Copy PDF #

Select All

Remove Rows

K2 Pt Cl4 - 00-009-0367

File Plots Help

Export Print

Wavelength: Cu K $\alpha$  1.54056 Å

2 $\theta$  (°)

2 $\theta$ (°)	d (Å)	I	h	k	l	*
12.59190	7.024000	1000	1	0	0	
17.84383	4.966720	102	1	1	0	
21.40901	4.147000	230	0	0	1	
24.91334	3.571050	390	1	0	1	
25.33913	3.512000	65	2	0	0	
28.00658	3.183270	521	1	1	1	
28.38920	3.141230	198	2	1	0	

PDF

Experimental

Physical

Crystal

Optical

Structure

Classifications

Cross-references

References

Comments

K2 (Pt Cl4) - 01-070-1408

File Plots Help

Export Print

Wavelength: Cu K $\alpha$  1.54056 Å

2 $\theta$  (°)

K2 (Pt Cl4) - 01-076-2175

File Plots Help

Export Print

Wavelength: Cu K $\alpha$  1.54056 Å

2 $\theta$  (°)

Intensity

1,000

800

600

400

200

0

10 20 30 40 50 60 70 80 90 100 110 120 130 140 15

2 $\theta$  (°)

Status: Alternate Quality Mark: Star

Environment: Ambient Temperature: 298.0 K (Assigned by ICDD editor) Pressure: -

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

Modification Date: 09/01/2016 Modifications: Quality

Open multiple PDF Cards.

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



Thank you for viewing our tutorial.  
Additional tutorials are available at the ICDD® website.  
[www.icdd.com](http://www.icdd.com)

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12 Campus Boulevard  
Newtown Square, PA 19073  
Phone: 610.325.9814  
Toll Free Number in US & Canada: 866.378.0331  
Fax: 610.325.9823