

PDF-2 TOOLS AND SEARCHES



PDF-2 2023

The PDF-2 2023 database is powered by our integrated search display software. PDF-2 2023 boasts 71 search selections coupled with 57 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 2023.

Tool Bar

PDF-2 2023
File Window Help

Open PDF Cards Preferences Search History Results Composition Graph Steve Microanalysis

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.
- ☐ 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 ☒ Boolean ☐ Yes/No/Maybe ☐ Composition List

And ☒ Or ☐ Not ☐ Grouping: ☒ And ☐ Or

Only ☐ Just ☐

Search Reset Tab Reset All

Range Input

Global Operator

Primary
Search Menu

Getting Started

PDF-2 2023

File Window Help

Open PDF Cards Preferences Search History Results Composition Graph Sieve Microanalysis

Select PDF Cards

PDF Number Sort by Most Recent

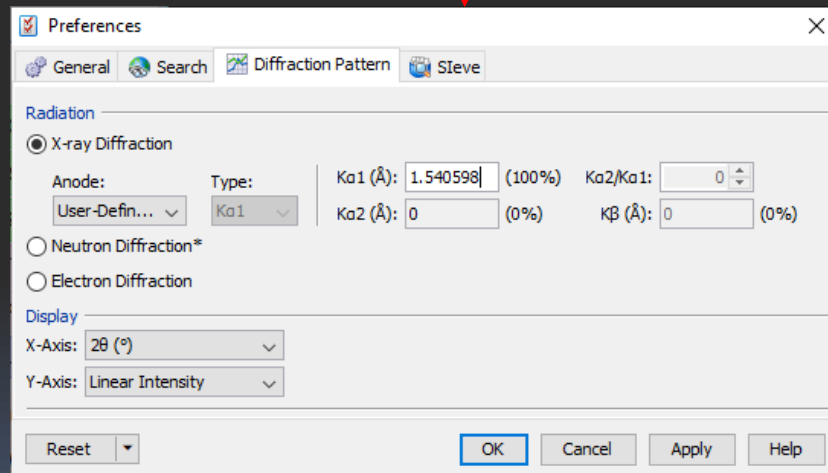
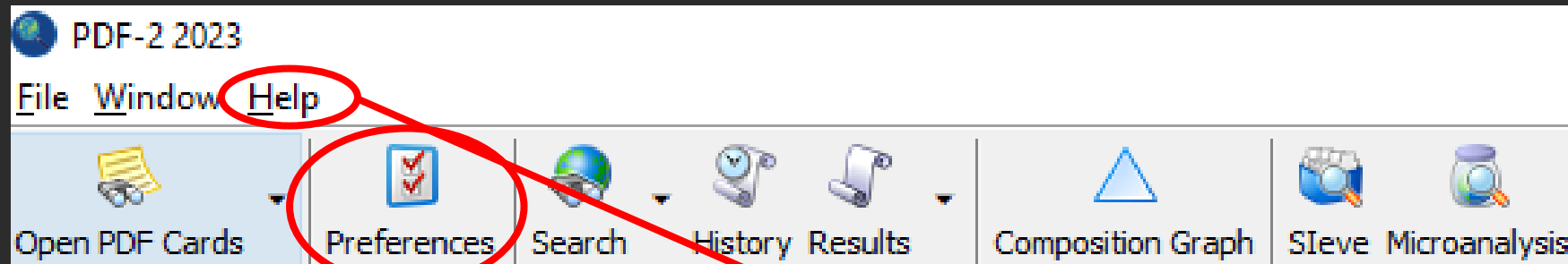
$C_{26}H_{27}F_3N_2O_6$ Tezacaftor 00-071-1635
$ZrH_2P_2O_8 \cdot H_2O$ Zirconium Hydrogen Phosphate Hydrate 00-071-0090
$((C_6H_7O_2)(C_2H_3O_2)_3)_n$ Cellulose triacetate I 00-064-1453
$Na(H_2PO_4)(H_2O)$ Sodium Hydrogen Phosphate Hydrate 01-070-0003

Clear List Open PDF Card Cancel

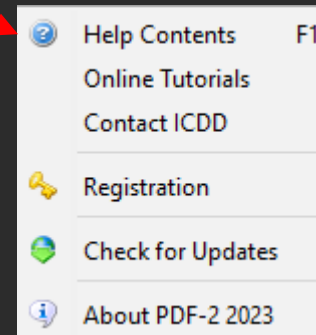
Open a known PDF card.

Navigate quickly to a recent PDF card.

Getting Started

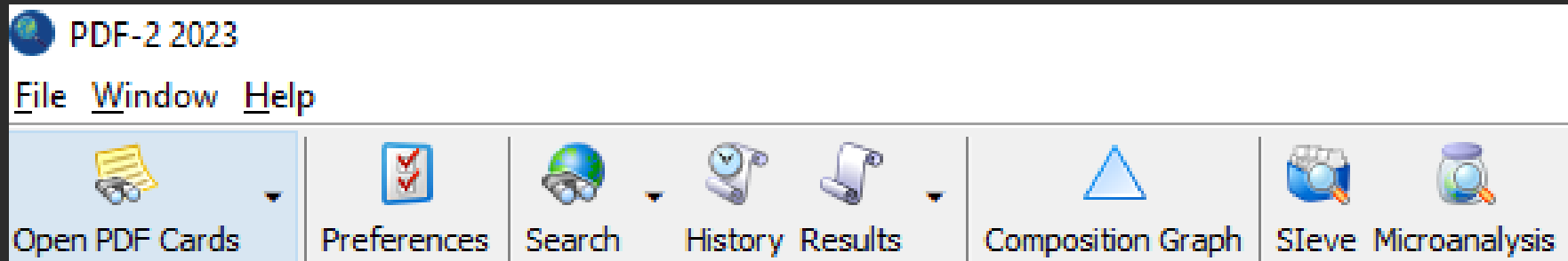


Customize Radiation, Display settings, and many more features of the PDF-2.



Help information regarding use, support, license policy, and registration of the PDF-2.

Tool Bar



Quick Navigation Icons



Open a PDF Card



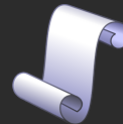
Select Preferences Module



Open Search Window



Open History Window



Open Results Window



Composition Graph



Open Sieve



Microanalysis

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:** 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, 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, and Minimal Acceptable, along with checkboxes for Blank, Low-Precision, and Hypothetical.
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05).
- Periodic Table:** A color-coded periodic table with element symbols and atomic numbers. It includes a search bar and radio buttons for Boolean, Yes/No/Maybe, and Composition List, as well as checkboxes for And, Or, Not, Only, and Just.
- Physical Properties:** A list of tabs including Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments.
- Range Input:** A section for entering search ranges 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

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

La: Ac:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

1 H 2 He

3 Li 4 Be

5 B 6 C 7 N 8 O 9 F 10 Ne

11 Na 12 Mg

13 Al 14 Si 15 P 16 S 17 Cl 18 Ar

19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr

37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe

55 Cs 56 Ba

57 La 58 Ce 59 Pr 60 Nd 61 Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy 67 Ho 68 Er 69 Tm 70 Yb 71 Lu

72 Hf 73 Ta 74 W 75 Re 76 Os 77 Ir 78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn

87 Fr 88 Ra

89 Ac 90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es 100 Fm 101 Md 102 No 103 Lr

Booleans: ☐ Boolean ☒ Yes/No/Maybe ☐ Composition List

Switch to No

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

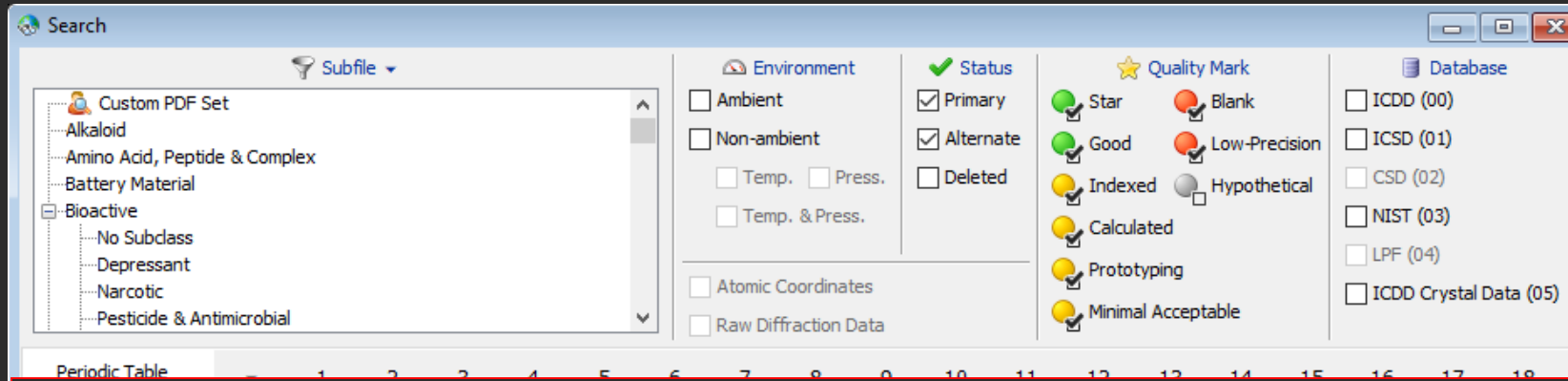
Search Reset Tab Reset All

Range 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. On the left, a tree view shows categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The main area features a periodic table with elements color-coded by group. Above the table, there are filter sections for 'Environment' (Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data), 'Status' (Primary, Alternate, Deleted), and 'Quality Mark' (Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Pre, Hypothetical). A search bar at the top right contains the text 'Boolean' and 'Yes, No, Maybe, Composition List'. Below the search bar, there are radio buttons for 'And', 'Or', 'Not', 'Only', and 'Just', and a 'Grouping' section with 'And' and 'Or' radio buttons. At the bottom, there are buttons for 'Search', 'Reset Tab', and 'Reset All', along with 'Range Input' and 'Global Operator' dropdown menus.

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
- 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:

Left sidebar: Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, Comments.

Search options: Boolean, Yes/No/Maybe (selected), Composition List.

Buttons: Search, Reset Tab, Reset All, 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).

Search Window

Subfile

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Bottom Material

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 Filters

☐ Boolean ☐ Yes/No/Maybe ☒ Composition List

Select 2-5 elements

Periodic Table

Search Results

Empirical Formula	Hits
Cl ₂	8
Cl ₄ Pt	3
Cl ₃ Pt	1
Cl ₂ Pt	9
Pt	53

La:
 Ac:

Range Input
 Global Operator

Search Reset Tab Reset All

Search Window

Formula/Name

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.

Number of Elements

Low High

Molecular Wt (g/mol)

Value ±Error

Composition

Element Weight % ±Error

Search Reset Tab Reset All

Range Input

Global Operator

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

Chemical Formula – filters based on the molecular formula.

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

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

Refined Formula – filters on a formula derived from the occupancies and site multiplicities of the elements in the atomic coordinates.

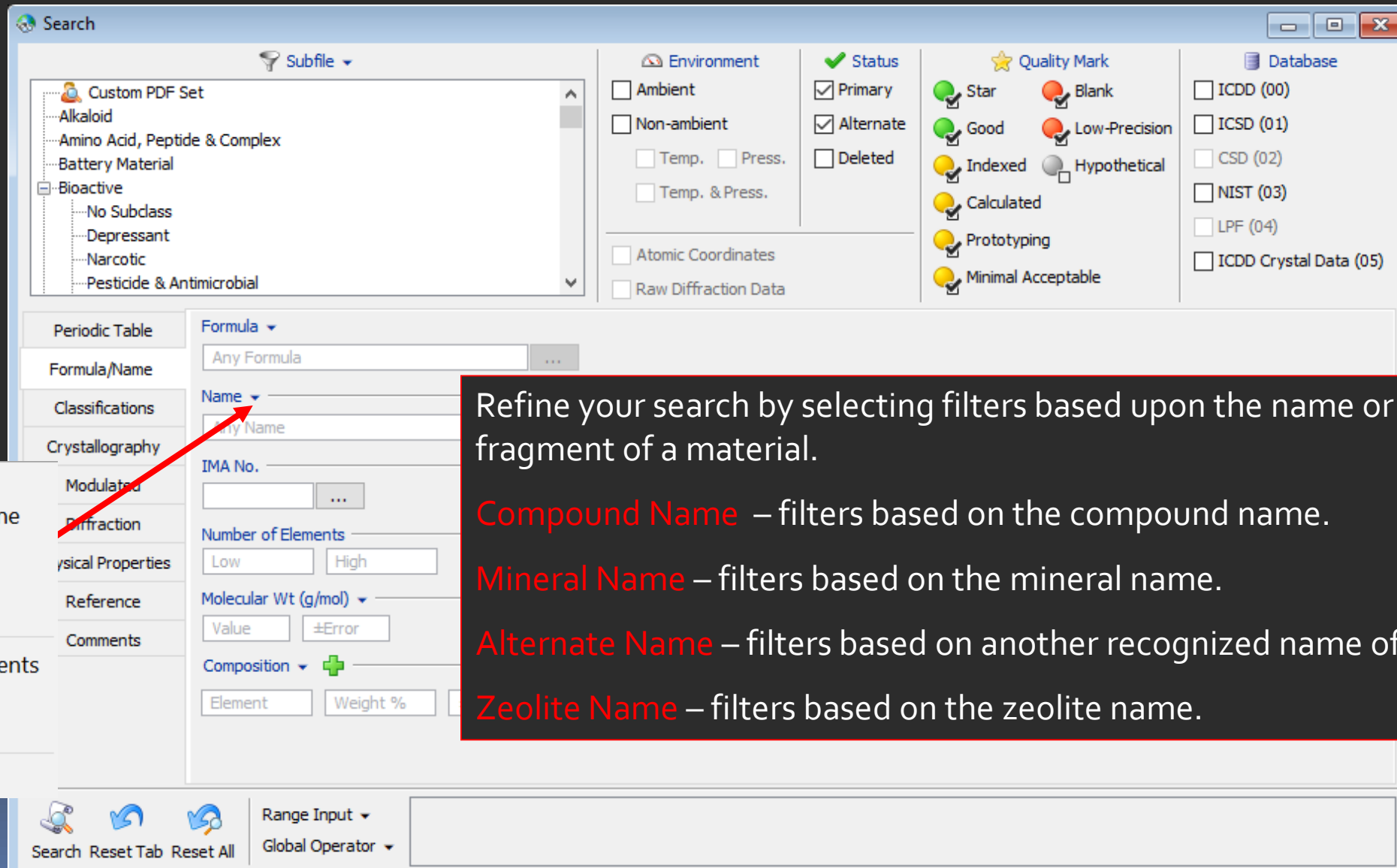
Number of Elements – filters on the total number of unique elements in a chemical formula.

Molecular Wt (g/mol) – filters based on molecular weight in g/mol

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

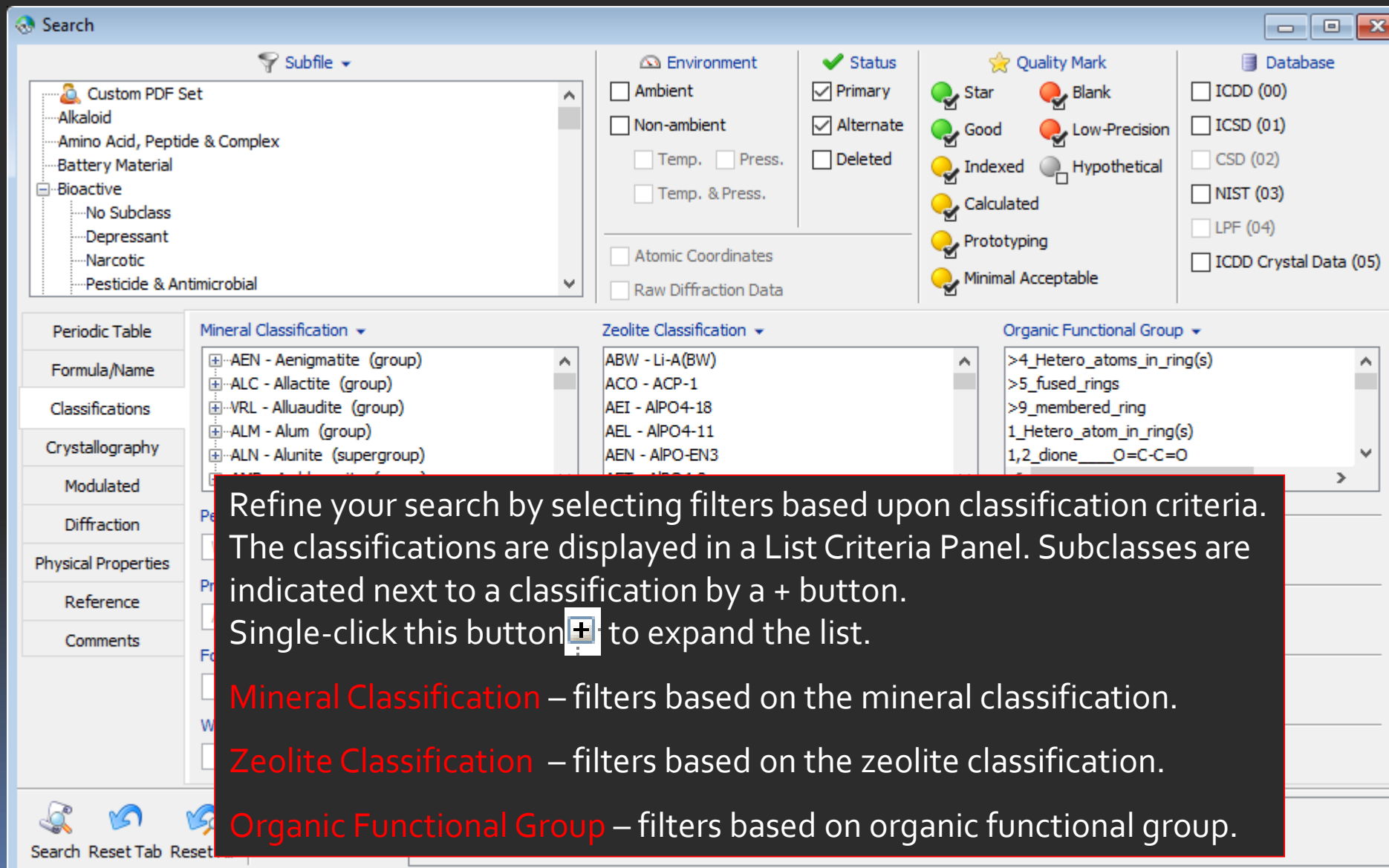
Search Window

Formula/Name




Search Window

Classifications



The screenshot displays the ICDD Search Window interface. On the left, a sidebar contains a tree view for 'Custom PDF Set' with categories like Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial. Below this is a 'Periodic Table' button and a list of search criteria: Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The main area is divided into several filter panels: '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 panels: 'Mineral Classification' (listing AEN - Aenigmatite, ALC - Allactite, VRL - Alluaudite, ALM - Alum, ALN - Alunite), 'Zeolite Classification' (listing ABW - Li-A(BW), ACO - ACP-1, AEI - AlPO4-18, AEL - AlPO4-11, AEN - AlPO-EN3), and 'Organic Functional Group' (listing >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). A red-bordered text box is overlaid on the bottom right of the window, containing instructions on how to refine searches using classification criteria.

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

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.
- ☐ 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

Mineral Classification

- AEN - Aenigmatite (group)
- ALC - Allactite (group)
- VRL - Alluaudite (group)
- ALM - Alum (group)
- ALN - Alunite (supergroup)
- AMB - Amblygonite (group)

Zeolite Classification

- ABW - Li-A(BW)
- ACO - ACP-1
- AEI - AlPO4-18
- AEL - AlPO4-11
- AEN - AlPO-EN3
- AET - AlPO4-8

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

Pearson Symbol

With Hydrogen

Prototype Structure

Any Prototype Structure

Formula Type (ANX)

Wyckoff Sequence

Range Input

Global Operator

Search Reset Tab Reset All

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Crystal System

- ☐ Triclinic
- ☐ Monoclinic
- ☐ Orthorhombic
- ☐ Tetragonal

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

Angles (°)

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume (Å³)

Value ±Error

Axial Ratio

c/a: Value ±Error

a/b: Value ±Error

c/b: Value ±Error

Search Reset Tab Reset All

Range Input

Global Operator

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

Search Window

Crystal Data

The screenshot shows the 'Search' window for 'Crystal Data'. The interface includes a left sidebar with a tree view of categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The main area contains several filter sections: '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), and 'Database' (ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05)). Below these are '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.)), and 'AET' (AET, Elements). A 'Space Group' dropdown menu is open, showing options: 'Space Group Symbol', 'Space Group Number', 'Aspect Symbol', 'Superspace Group Symbol', 'Contains Fragments', 'Contains Phrase Exactly', and 'Not'. Red arrows point from callout boxes to these options. The bottom of the window has a 'Search' button, 'Reset Tab', 'Reset All', and a 'Global Operator' dropdown.

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

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

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

Crystal (Symmetry Allowed)

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

AET

AET

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

Angles (°)

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume (Å³)

Value ±Error

Axial Ratio

c/a: Value ±Error

a/b: Value ±Error

c/b: Value ±Error

Search Reset Tab Reset All

Global Operator

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

Filters based on the volume 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

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

☐ Triclinic (Anorthic) ☐ Rhombohedral

☐ Monoclinic ☐ Hexagonal

☐ Orthorhombic ☐ Cubic

☐ Tetragonal

Crystal (Symmetry Allowed)

☐ Centrosymmetric

☐ Non-centrosymmetric:

☐ Enantiomorphic ☐ Pyro / Piezo (p)

☐ Optical Activity ☐ Piezo (2nd Harm.)

AET

AET

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

Angles (°)

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume (Å³)

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

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Convert Cell

Crystal System:

Bravais Lattice:

☒ Convert to Crystal Data

☐ Convert to Reduced Cell

Convert Cancel

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Space Group

Space Group Symbol

Crystal Data Reduced Cell Author's Unit Cell Supercell/Subcell

Axis (Å)

a:

b:

c:

Angles (°)

α:

β:

γ:

Volume (Å³)

Value

Molecular/f.u. Volume

Value

Axial Ratio

a/b:

c/b:

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 Reset Tab Reset All

Range Input

Global Operator

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 to the 'Supercell/Subcell' tab 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 (Symmetry Allowed):** Centrosymmetric, Non-centrosymmetric, Enantiomorphic, Pyro / Piezo (p), Optical Activity, Piezo (2nd Harm.)
- Space Group:** Space Group Symbol
- Crystal Data:** Reduced Cell, Author's Unit Cell, **Supercell/Subcell**
- Axis (Å):** a, b, c (Value, ±Error)
- Angles (°):** α, β, γ (Value, ±Error)
- Supercell/Subcell:** Supercell (selected), Subcell, Volume Ratio: 1 to 1

At the bottom, there are icons for Search, Reset Tab, and Reset All, along with Range Input and Global Operator dropdowns.

Search Window

Modulated

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ D

Quality Mark

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

Database

- ☐ ICDD (00)
- ☐ ICSD (01)
- ☐ ICDD Crystal Data (05)

Modulated Dimension

- ☐ 3 + 1d
- ☐ 3 + 2d
- ☐ 3 + 3d

Subsystems

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

Range Input

Global Operator

Search Reset Tab Reset All

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
- ☐ 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

Radiation: ☒ X-ray/Electron ☐ CW Neutron

Strong Line (Å)

D1 D2 D3

Value Value Value ±Error

Long Line (Å)

L1 L2 L3

Value Value 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

Range Input

Global Operator

Search Reset Tab Reset All

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
- ☐ 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

☐ Property Sheet ☐ Topology Data

Topology

Topology vdW Volume (Å³)

Value ±(%)

Topology Total Porosity (Å)

Value ±(%)

Topology vdW Surface Area (Å²)

Value ±(%)

Color

- ☒ Black
- ☐ Blue
- ☐ Brown
- ☐ Color Missing
- ☐ Colorless

Kelvin (K)

Celsius (°C)

Fahrenheit (°F)

Not

Search Reset Tab Reset All

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 ICDD Search window. On the left is a sidebar with a tree view of material classes (Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, etc.) and a list of search criteria (Periodic Table, Formula/Name, Classifications, Crystallography, etc.). The 'Reference' criterion is selected. The main search area contains fields for Author, Title, Publication, Year (Start/End), and DOI. A red box highlights the 'Publication' dropdown menu, which is open, showing options: 'Journal/Patent CODEN', 'Contains Fragments', 'Contains Phrase', 'Exactly', and 'Not'. A red arrow points from the text in the red box to the 'Publication' dropdown. The text in the red box explains how to refine the search by selecting filters based on journal references and lists the available filter options.

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

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:

Search Reset Tab Reset All

Range Input

Global Operator

ICDD

INTERNATIONAL CENTER FOR DIFFRACTION DATA

ISO 9001:2015

QUALITY MANAGEMENT SYSTEM CERTIFIED

BY DEKRA

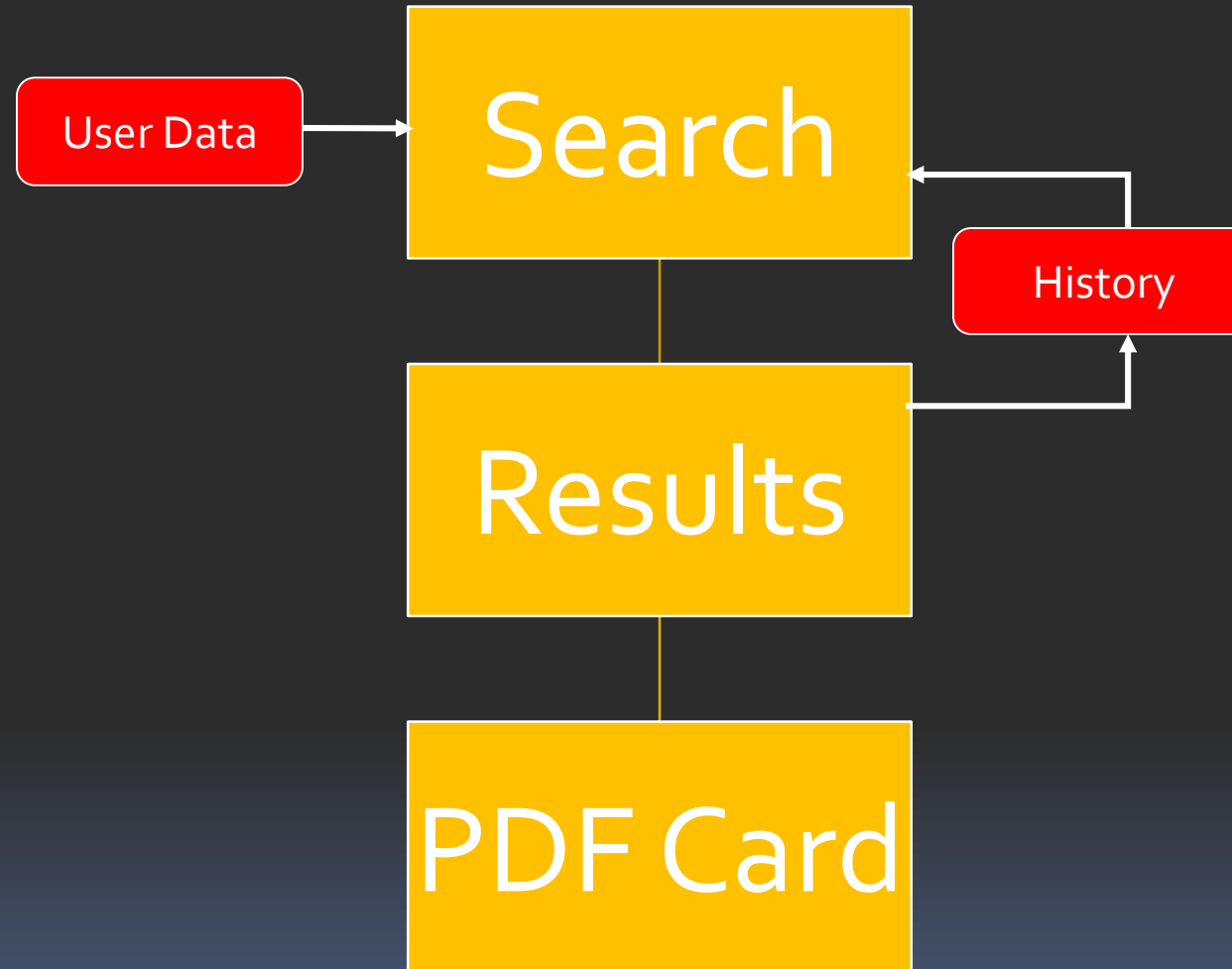
CEP 110

110409 01

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.



Select
Elements in
Periodic Table

Search Example

The image displays three screenshots of the ICDD search interface, illustrating the steps to select elements, a space group, and a compound name.

Top Screenshot: Shows the search criteria panel. The "Periodic Table" tab is selected. The "Formula/Name" field is empty. The "Classifications" field is set to "Boolean". The "Crystallography" field is set to "And". The "Status" field is set to "Primary". The "Quality Mark" field is set to "Star". The "Database" field is set to "ICDD (00)".

Bottom Left Screenshot: Shows the search criteria panel. The "Periodic Table" tab is selected. The "Formula/Name" field is empty. The "Classifications" field is set to "Boolean". The "Crystallography" field is set to "And". The "Status" field is set to "Primary". The "Quality Mark" field is set to "Star". The "Database" field is set to "ICDD (00)". The "Space Group" field is set to "P4/mmm".

Bottom Right Screenshot: Shows the search criteria panel. The "Periodic Table" tab is selected. The "Formula/Name" field is empty. The "Classifications" field is set to "Boolean". The "Crystallography" field is set to "And". The "Status" field is set to "Primary". The "Quality Mark" field is set to "Star". The "Database" field is set to "ICDD (00)". The "Name" field is set to "Potassium Platinum Chloride".

Selected filters highlighted in red:

- Periodic Table
- Formula/Name
- Classifications
- Crystallography
- Space Group
- Name
- Potassium Platinum Chloride

Select Space Group

Select Compound Name

Selected filters highlighted in red

Search Results

Results - 8 of 339,549

File Fields Tools

Open PDF Card Simulated Profile My Defaults

PDF #	QM	Chemical Formula	Con	D1 (Å)	D2 (Å)	D3 (Å)	SYS
00-009-0367	● I	K_2PtCl_4	Potassium Platinum Chloride	6.940	3.160	3.550	T
01-070-1408	● I	K_2PtCl_4	Potassium Platinum Chloride	7.027500	3.182740	3.569850	T
01-073-1506	● I	$K_2(PtCl_4)$	Potassium Platinum Chloride	6.990000	3.169250	3.555730	T
01-074-1616	● I	$K_2(Pt(CN)_4)Cl_{0.32}(H_2O)_{2.6}$	Potassium Platinum Chloride Cyanide Hydrate	9.866000	4.412210	6.976320	T
01-076-2175	● S	$K_2(PtCl_4)$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T
01-077-1947	● S	K_2PtCl_4	Potassium Platinum Chloride	7.023000	3.183810	3.571940	T
01-080-0953	● S	$K_2(PtCl_4)$	Potassium Platinum Chloride	6.996100	3.159080	3.540590	T
01-080-0954	● S	$K_2(PtCl_4)$	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 [Exclude Deleted/Hypothetical Patterns]

Search Results

Search Filters

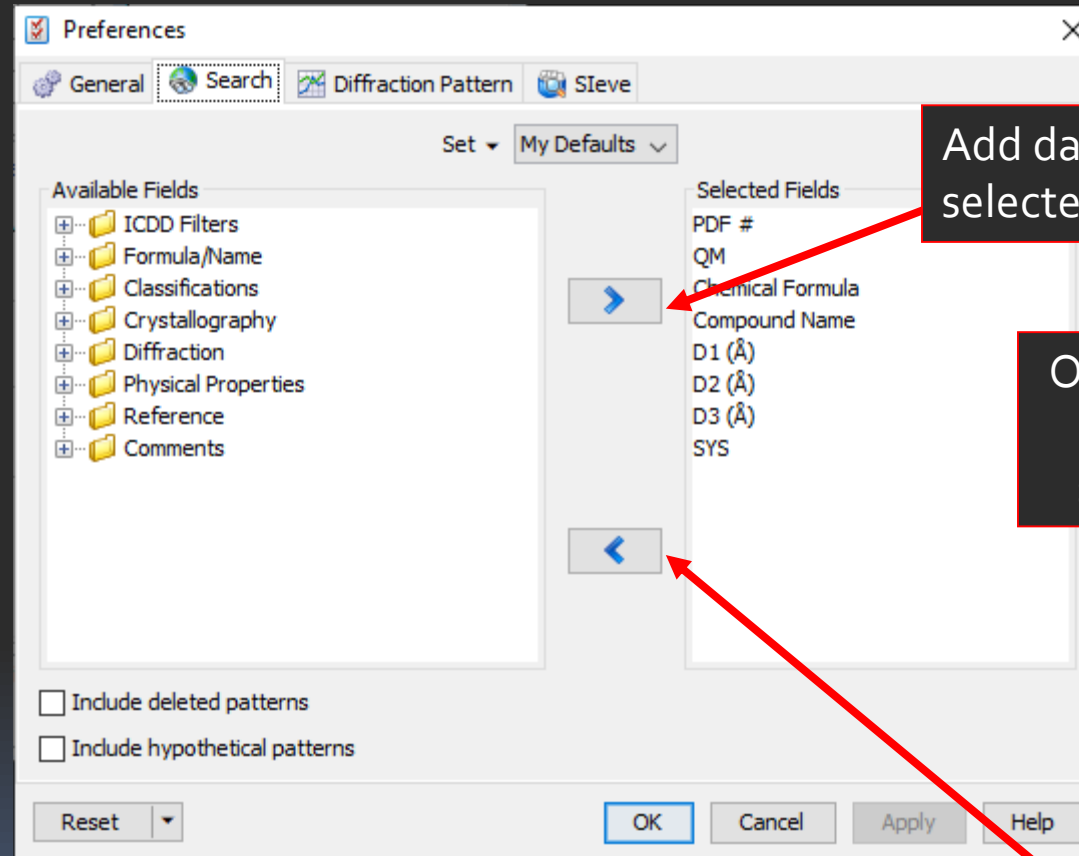
Double-click on a PDF number to view the entire PDF Card.



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.



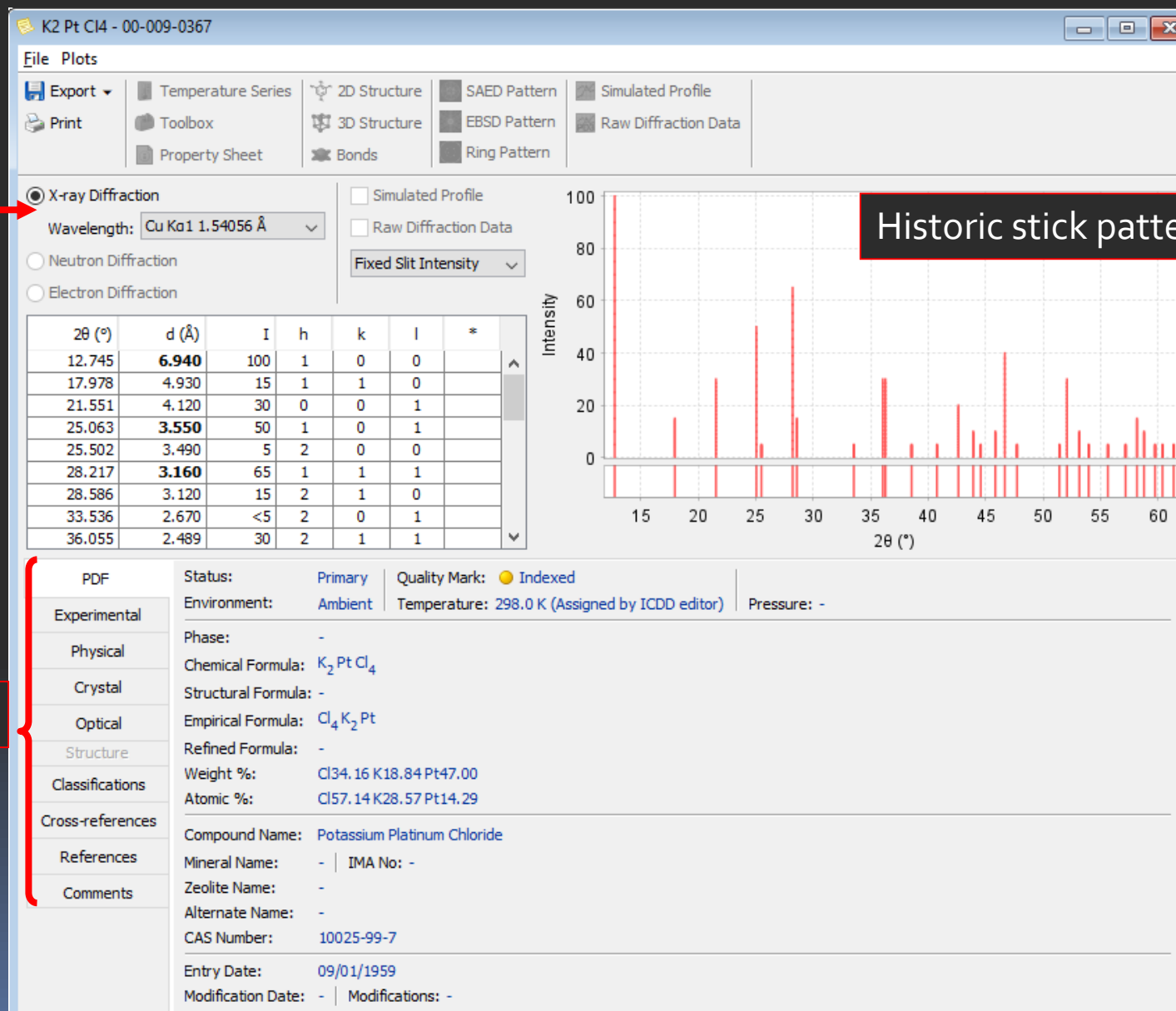
Add data fields to selected list

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 339,549

File Fields Tools

Open PDF Card Simulated Profile

PDF #	QM	Chemical Formula	Compound Name
00-009-0367	● I	K_2PtCl_4	in Chloride
01-070-1408	● I	K_2PtCl_4	in Chloride
01-073-1506	● I	$K_2(PtCl_4)$	in Chloride
01-074-1616	● I	$K_2(PtCl_4)$	in Chloride
01-076-2175	● S	$K_2(PtCl_4)$	in Chloride
01-077-1947	● S	K_2PtCl_4	in Chloride
01-080-0953	● S	$K_2(PtCl_4)$	in Chloride
01-080-0954	● S	$K_2(PtCl_4)$	in Chloride

Open PDF Card

Tools/Simulations

Add to Custom PDF Set...

Remove from Custom PDF Set...

Copy Chemical Formula

Remove Rows

[[Pt And Cl]] And [Any Name Co
[P4/mmm]] And [Exclude Deleted
[hypocenter atoms]]

Open multiple PDF Cards.

old the Ctrl
y, then
lect PDF
rds. Right
ck mouse,
ect Open
DF Card.

K2 Pt Cl4 - 00-009-0367

File Plots

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

K2 Pt Cl4 - 01-070-1408

File Plots

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

K2 (Pt Cl4) - 01-076-2175

File Plots

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

Toolbox 3D Structure EBSD Pattern Raw Diffraction Data

Property Sheet Bonds Ring Pattern

Wavelength: Cu Ko1 1.54056 Å

Wavelength: 2θ (°)

Intensity

2θ (°)	d (Å)	I	h	k	l	*
12.592	7.024000	1000	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	
28.389	3.141230	198	2	1	0	
33.406	2.680060	8	2	0	1	
35.832	2.503980	198	2	1	1	

PDF

Experimental

Physical

Crystal

Optical

Structure

Classifications

Cross-reference

References

Comments

Status: Primary Quality Mark: Star

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

Phase: -

Chemical Formula: $K_2(PtCl_4)$

Structural Formula: -

Empirical Formula: Cl_4K_2Pt

Refined 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: -

Zeolite Name: -

Alternate Name: potassium tetrachloroplatinate(II)

CAS Number: -

Entry Date: 09/01/1998

Modification Date: 09/01/2020 Modifications: Update



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

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Newtown Square, PA 19073
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Toll Free Number in US & Canada: 866.378.0331
Fax: 610.325.9823