

# PDF-4+ Tools and Searches



# PDF-4+ 2019

The PDF-4+ 2019 database is powered by our integrated search display software. PDF-4+ 2019 boasts 74 search selections coupled with 126 display fields resulting in a nearly limitless choice of data mining options. This quick tutorial will introduce you to the basics of PDF-4+ filters available to you to refine your search.

Getting Started: The Toolbar

Search Window: Overview of Search Classifications

Data Mining Basics

Search Example

Preferences Module

PDF Data Card

# Launch Screen

This will be the opening screen when you have correctly opened PDF-4+ 2019.

PDF-4+ 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

Boolean Yes/No/Maybe Composition Diagram List

And Or Not

Only Just

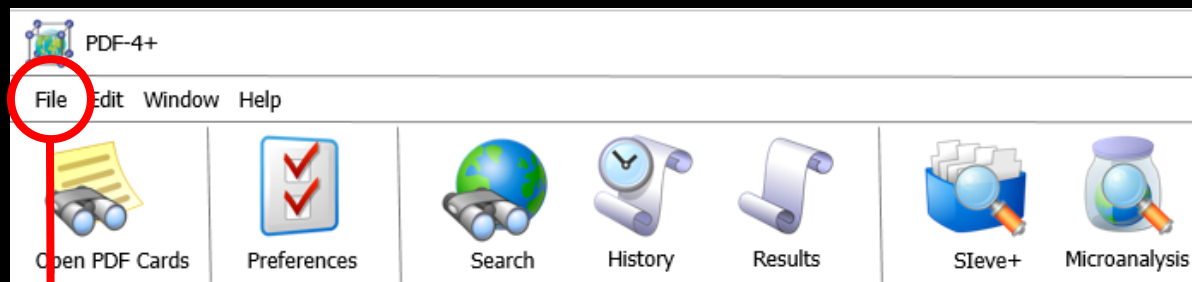
Grouping: And Or

Search Reset Tab Reset All Help Range Input Global Operator

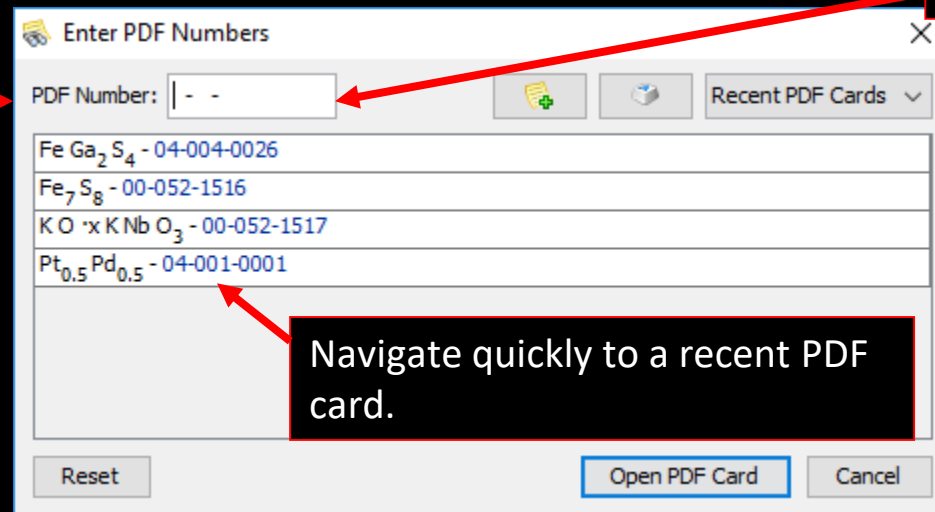
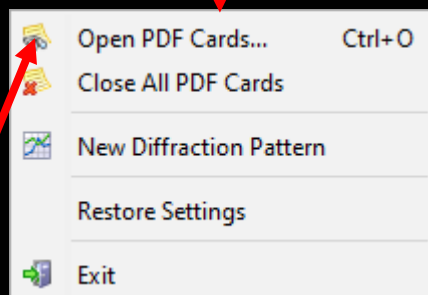
Tool Bar

Primary Search Menu

# Getting Started

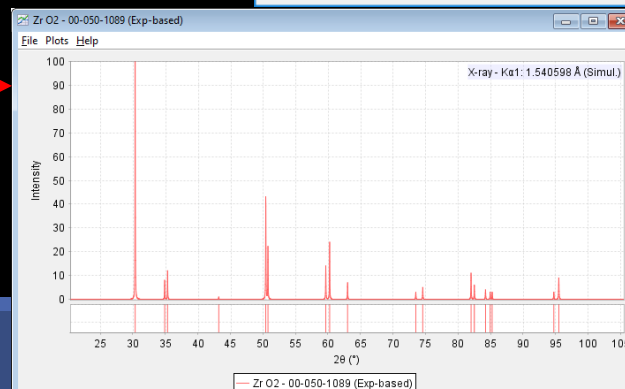


Open a known PDF card.

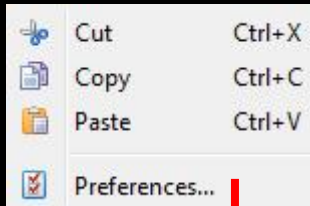
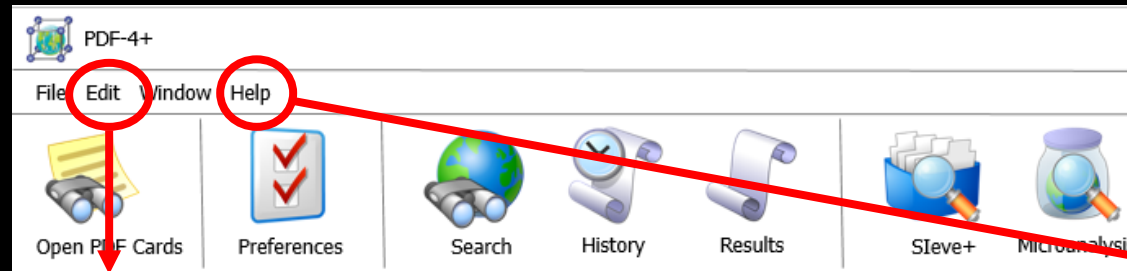


Navigate quickly to a recent PDF card.

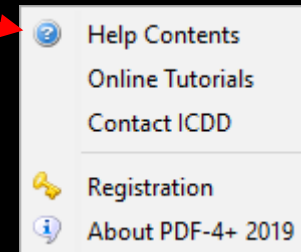
Open a previously saved diffraction pattern. The pattern must be of the ICDD XML file format. All PDF entries can be saved in this format.



# Getting Started

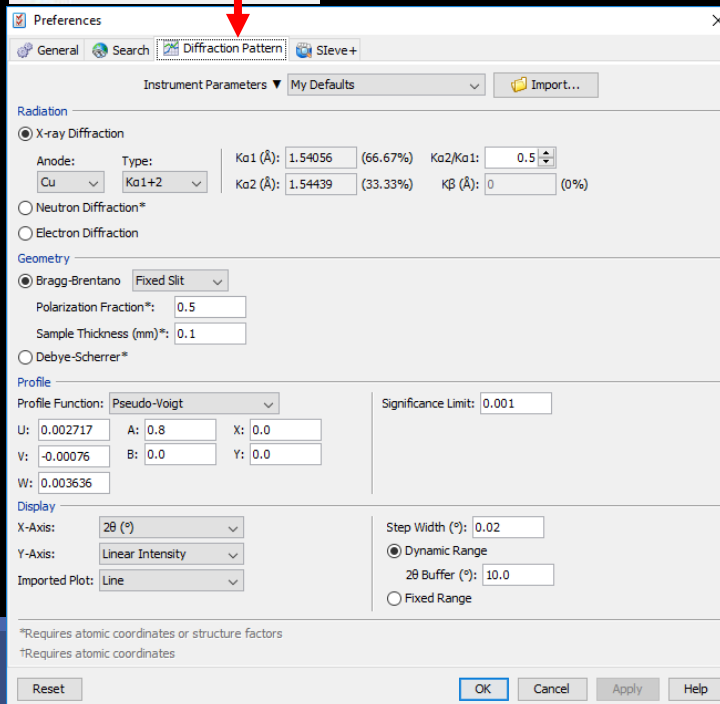


Edit functions

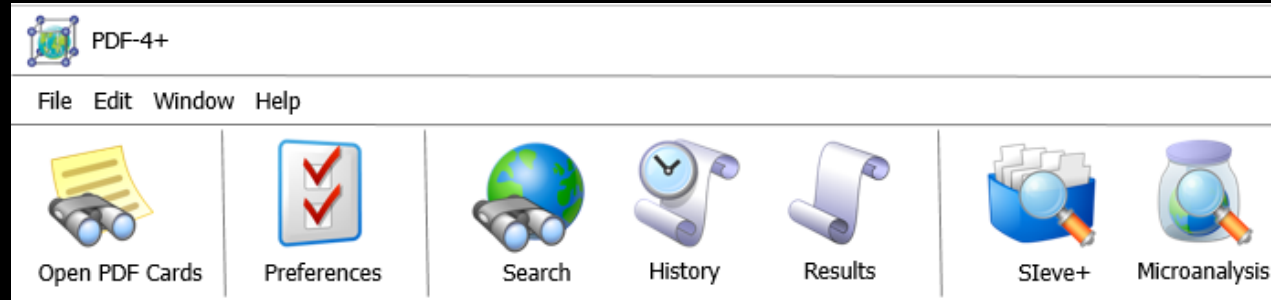


Help information regarding use, support, license policy, and registration of the PDF-4+. Be sure to register the PDF-4+ upon installation to activate the full license term.

Customize Radiation, Geometry, Profile, Display settings and many more features of the PDF-4+.



# 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-4+. Searching the PDF-4+ is an iterative process that allows you to input user-defined criteria, view the results, and combine additional criteria to refine your results.

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

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H 1.008																	He 4.003
2	Li 6.941	Be 9.012											B 10.811	C 12.01	N 14.007	O 15.999	F 18.998	Ne 20.180
3	Na 22.990	Mg 24.305											Al 26.982	Si 28.086	P 30.974	S 32.065	Cl 35.453	Ar 39.948
4	K 39.098	Ca 40.078	Sc 44.956	Ti 47.867	V 50.941	Cr 51.996	Mn 54.938	Fe 55.845	Co 58.933	Ni 58.693	Cu 63.546	Zn 65.409	Ga 69.723	Ge 72.64	As 74.922	Se 78.96	Br 79.904	Kr 83.798
5	Rb 85.468	Sr 87.62	Y 88.906	Zr 91.224	Nb 92.906	Mo 95.94	Tc 98	Ru 101.07	Rh 102.906	Pd 106.42	Ag 107.868	Cd 112.41	In 114.818	Sn 118.71	Sb 121.76	Te 127.6	I 126.904	Xe 131.293
6	Cs 132.905	Ba 137.327		Hf 178.49	Ta 180.948	W 183.84	Re 186.207	Os 190.23	Ir 192.217	Pt 195.078	Au 196.967	Hg 200.59	Tl 204.383	Pb 207.2	Bi 208.98	Po [209]	At [210]	Rn [222]
7	Fr [223]	Ra [226]		Rf [261]	Db [262]	Sg [266]	Bh [264]	Hs [277]	Mt [268]	Ds [271]	Rg [272]	Cn [285]	Nh [286]	Fl [289]	Mc [289]	Lv [293]	Ts [294]	Og [294]
La			La 138.905	Ce 140.116	Pr 140.908	Nd 144.242	Pm [145]	Sm 150.36	Eu 151.964	Gd 157.25	Tb 158.925	Dy 162.5	Ho 164.93	Er 167.259	Tm 168.934	Yb 173.04	Lu 174.967	
Ac			Ac [227]	Th 232.038	Pa 231.036	U 238.029	Np [237]	Pu [244]	Am [243]	Cm [247]	Bk [247]	Cf [251]	Es [252]	Fm [257]	Md [258]	No [259]	Lr [262]	

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Boolean Yes/No/Maybe Composition Diagram List

And Or Not

Grouping: And Or

Search

Reset Tab

Reset All

Help

Range Input ▼ Global Operator ▼

# Search Window

## Subfiles/Database Filters

Search

Subfile ▼

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

Grouping: ☐ And ☐ Or

Search

Reset Tab

Reset All

Help

Range Input ▼ Global Operator ▼

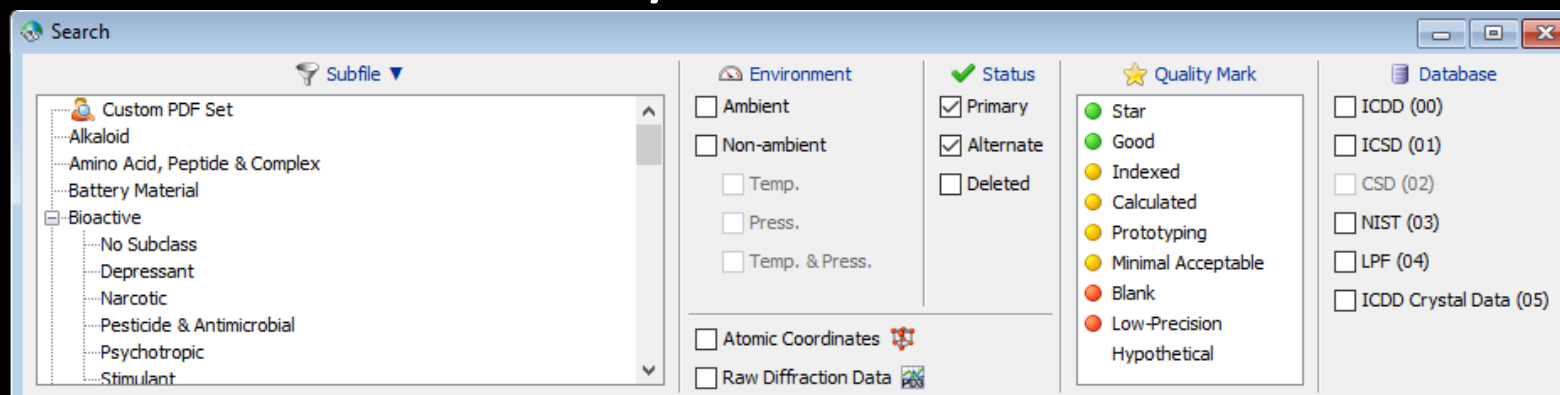
Refine your search by selecting filters.  
Select criteria under **Subfile**, **Environment**, **Status**, **Atomic Coordinates**, **Raw Diffraction Data (PD3)**, **Quality Mark (QM)**, and **Database**.





# 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).

**Atomic Coordinates** – filters based on entries that contain atomic coordinates or a cross-reference to an entry with atomic coordinates.

**Raw Diffraction Data (PD3)** – filters based on entries with high quality raw experimental data that can consist of nano-crystalline materials, semi-crystalline materials, or amorphous materials.

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

**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

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

ICDD (0)

ICSD (0)

CSD (02)

NIST (00)

LPF (04)

ICDD Cr

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

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

1 H 1.008

2 Li 6.941 4 Be 9.012

3 Na 22.990 12 Mg 24.305

4 K 39.098 20 Ca 40.078 21 Sc 44.956 22 Ti 47.867 23 V 50.941 24 Cr 51.996 25 Mn 54.938 26 Fe 55.845 27 Co 58.933 28 Ni 58.693 29 Cu 63.546 30 Zn 65.409 31 Ga 69.723 32 Ge 72.64 33 As 74.922 34 Se 78.96 35 Br 79.904 36 Kr 83.798

5 Rb 85.468 38 Sr 87.62 39 Y 88.906 40 Zr 91.224 41 Nb 92.906 42 Mo 95.94 43 Tc [98] 44 Ru 101.07 45 Rh 102.906 46 Pd 106.42 47 Ag 107.868 48 Cd 112.41 49 In 114.818 50 Sn 118.71 51 Sb 121.76 52 Te 127.6 53 I 126.904 54 Xe 131.293

6 Cs 132.905 56 Ba 137.327 72 Hf 178.49 73 Ta 180.948 74 W 183.84 75 Re 186.207 76 Os 192.227 77 Ir 192.227 78 Pt 195.078 79 Au 196.967 80 Hg 200.59 81 Tl 204.383 82 Pb 207.2 83 Bi 208.98 [209] 84 Po [209] 85 At [210] 86 Rn [222]

7 Fr [223] 88 Ra [226] 104 Rf [261] 105 Db [262] 106 Sg [266] 107 Bh [264] 108 Hs [277] 109 Mt [268] 110 Ds [271] 111 Rg [285] 112 Cn [285] 113 Nh [286] 114 Fl [289] 115 Mc [289] 116 Lv [293] 117 Ts [294] 118 Og [294]

La 138.906 57 La 138.906 58 Ce 140.116 59 Pr 140.908 60 Nd 144.242 61 Pm [145] 62 Sm 150.36 63 Eu 151.964 64 Gd 157.25 65 Tb 158.925 66 Dy 162.5 67 Ho 164.93 68 Er 167.259 69 Tm 168.934 70 Yb 173.04 71 Lu 174.967

Ac 232.038 89 Ac 232.038 90 Th 231.036 91 Pa 231.036 92 U 238.029 93 Np [237] 94 Pu [244] 95 Am [243] 96 Cm [247] 97 Bk [247] 98 Cf [251] 99 Es [252] 100 Fm [257] 101 Md [258] 102 No [259] 103 Lr [262]

Boolean Yes/No/Maybe Composition Diagram List

And Or Not

Grouping: + -

Only Just

And Or

Search

Reset Tab

Reset All

Help

Range Input ▼ 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.

**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: [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 ICDD Search Window with the Periodic Table Filters section expanded. The filters include Environment (Ambient, Non-ambient, Temp., Press., Temp. & Press.), 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)). The Composition Diagram List is selected, showing a list of phases sorted by empirical formula. The list includes Fe, Fe<sub>0.95</sub>Ni<sub>0.05</sub>, Fe<sub>0.9463</sub>Ni<sub>0.0537</sub>, Fe<sub>0.946</sub>Ni<sub>0.054</sub>, Fe<sub>0.9458</sub>Ni<sub>0.0542</sub>, Fe<sub>0.9441</sub>Ni<sub>0.0559</sub>, Fe<sub>0.9429</sub>Ni<sub>0.0571</sub>, Fe<sub>0.94</sub>Ni<sub>0.06</sub>, Fe<sub>0.9381</sub>Ni<sub>0.0619</sub>, Fe<sub>0.92</sub>Ni<sub>0.08</sub>, Fe<sub>0.916</sub>Ni<sub>0.084</sub>, Fe<sub>10.8</sub>Ni, Fe<sub>0.91</sub>Ni<sub>0.09</sub>, Fe<sub>0.9</sub>Ni<sub>0.1</sub>, Fe<sub>0.8782</sub>Ni<sub>0.1218</sub>, Fe<sub>0.8434</sub>Ni<sub>0.1566</sub>, and Fe<sub>5</sub>Ni. The hits are 131, 4, 1, 1, 1, 1, 1, 2, 1, 1, 24, 1, 2, 2, 2, and 1 respectively. The Search button is highlighted.

# Search Window

## Formula/Name

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 Window Interface:

- 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).
- Formula/Name:** Any Formula, Name (Any Name), IMA No., CAS Number, Number of Elements (Low/High), Composition (Element/Weight %), Error.

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

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

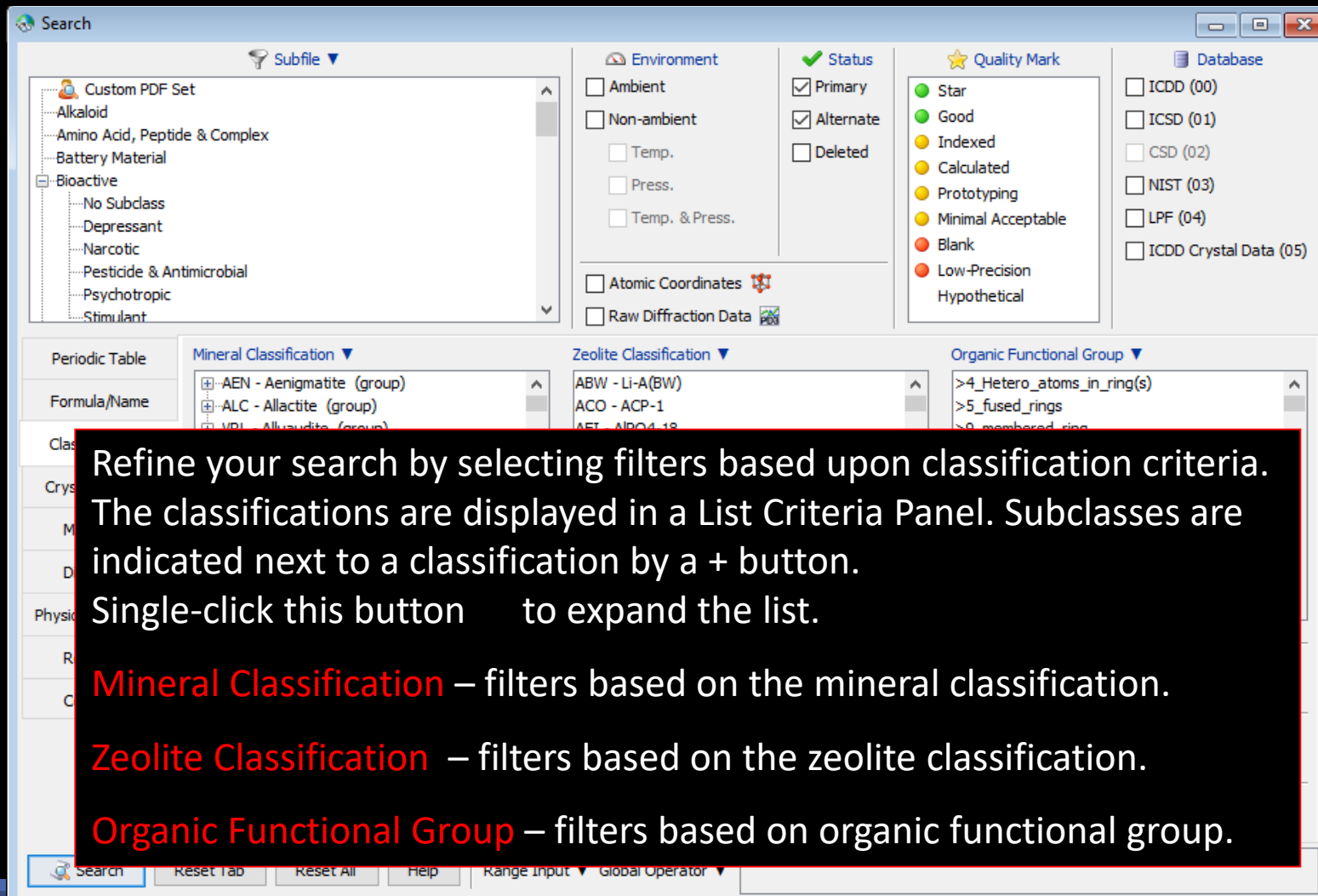
**Mineral Name** – filters based on the mineral name.

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

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

# Search Window

## Classifications



The screenshot shows the ICDD Search Window with several filter panels. The 'Subfile' panel on the left lists categories like Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, and Stimulant. 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 features a list of quality indicators: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, and Hypothetical. The 'Database' panel lists ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05). Below these are three classification panels: 'Mineral Classification' (showing AEN - Aenigmatite, ALC - Allactite, and VPI - Alluvialite), 'Zeolite Classification' (showing ABW - Li-A(BW), ACO - ACP-1, and AET - APO-18), and 'Organic Functional Group' (showing >4\_Hetero\_atoms\_in\_ring(s), >5\_fused\_rings, and >9\_membered\_ring). A red-bordered text box is overlaid on the bottom half of the window, providing instructions on how to refine searches using these 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
  - 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

Mineral Classification ▼

- ☒ AEN - Aenigmatite (group)
- ☒ ALC - Allactite (group)
- ☒ VRL - Alluaudite (group)
- ☒ ALM - Alum (group)
- ☒ ALN - Alunite (supergroup)
- ☒ AMB - Amblygonite (group)
- ☒ AMP - Amphibole (family)
- ☒ ANC - Analcime (supergroup)
- ☒ ANY - Ancyrite (supergroup)
- ☒ ADA - Andalusite (group)
- ☒ ANT - Antlerite (group)

Zeolite Classification ▼

- 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
- AFR - SAPO-40

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\_ring

Pearson Symbol ▼

With Hydrogen

Prototype Structure ▼

Any Prototype Structure

Formula Type (ANX) ▼

Search

Reset Tab

Reset All

Help

Range Input ▼ Global Operator ▼

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
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  - Psychotropic
  - Stimulant

Environment

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

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- ☒ Low-Precision
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Database

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- ☐ 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
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

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

axial Ratio

a/b: Value ± Error

c/b: 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 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
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

Space Group ▼

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

Volume

Value

± Error

Search

Reset Tab

Reset All

Help

Range Input ▼

Global Operator ▼

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

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

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

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

# Search Window

## Crystal Data

Search

Subfile ▼

Custom PDF Set

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

☐ 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

1#a 2#a 2#b 3#a 3#b

Ac Ag Al Am Ar

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 ▼

Filters based on the volume of the crystal data.

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

# Search Window

## Reduced Cell

Search

Subfile ▼

Custom PDF Set

- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
  - No Subclass
  - Depressant
  - Narcotic
  - Pesticide & Antimicrobial
  - 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
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

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 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

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)

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal Data

Reduced Cell

Author's Unit Cell

Supercell/Subcell

Space Group ▼

Space Group Symbol

Tridinic (Anorthic) ☐ Rhombohedral ☐ Centrosymmetric ☐

Monoclinic ☐ Hexagonal ☐ Non-centrosymmetric: ☐

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

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

Axis (Å)

Convert Cell for Search...

b: Value ± Error β: Value ± Error

c: Value ± Error γ: Value ± Error

Volume

Value ± Error

Molecular/f.u. Volume

Value ± Error

Convert Cell

Author's Crystal System: Tridinic (Anorthic) ▼

Author's Lattice Centering: Primitive ▼

Cell Type: Crystal ▼

Convert Cancel

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 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. The left sidebar contains a list of search categories: Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, and others. The main area is divided into several sections: Environment (Ambient, Non-ambient, Temp., Press., Temp. & Press.), 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 sections for Crystal (Symmetry Allowed) and Atomic Environment Type. The bottom section is titled 'Supercell/Subcell' and contains a 'Space Group' dropdown, a 'Space Group Symbol' input field, and a table for 'Axis (Å)' with columns for 'a', 'b', 'c' and 'Value', '± Error'. The 'Supercell' radio button is selected, and the 'Volume Ratio' is set to 1 to 1. A red arrow points from the text box to the 'Supercell/Subcell' section.

Search

Subfile

Custom PDF Set

Alkaloid

Amino Acid, Peptide & Complex

Environment

Ambient

Non-ambient

Temp.

Press.

Temp. & Press.

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.)

Atomic Environment Type

Symbol

Elements

1#a

2#a

2#b

3#a

3#b

Ac

Ag

Al

Am

Ar

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

Supercell

Volume Ratio: 1 to 1

Subcell

Search

Reset Tab

Reset All

Help

Range Input

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

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
- ☐ Deleted

Quality Mark

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

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)

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

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.

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

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)

Radiation: ☒ X-ray/Electron ☐ CW Neutron

Strong Line (Å) ▼

Value  ± Error

Long Line (Å) ▼

Value  ± Error

☒ D1 ☒ D2 ☒ D3

☒ L1 ☒ L2 ☒ L3

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 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/cm<sup>3</sup>) ▼

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

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 Ref

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 ▼

Absolute Configuration

Additional Diffraction Lines

Additional Patterns

Analysis

ANX

Atomic Position

Bioactivity

Boiling Point

Calculated Pattern Original Remarks

Search

Reset Tab

Reset All

Help

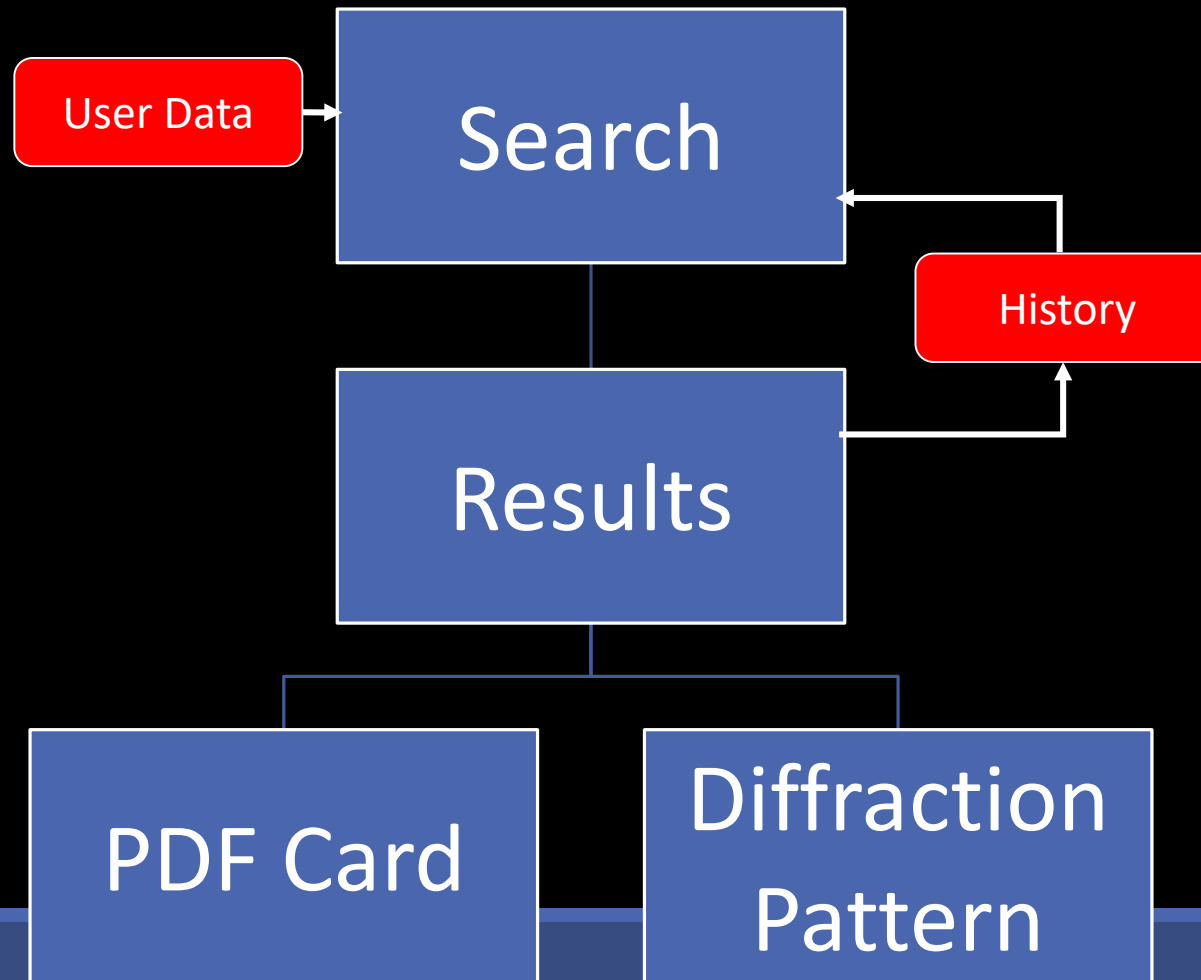
Range Input ▼ Global Operator ▼

Filter based on the text contained in comments.

# 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

This screenshot shows the top portion of the ICDD search interface. On the left, a tree view for 'Custom PDF Set' includes categories like Alkaloid, Amino Acid, Peptide & Complex, Battery Material, and Bioactive. The 'Bioactive' category is expanded, showing sub-classes such as No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial, Psychotropic, and Stimulant. A red arrow points from the 'Select Elements in Periodic Table' text to the periodic table, which is currently displaying elements from Hydrogen (H) to Xenon (Xe). To the right of the periodic table are several filter panels: 'Environment' (Ambient, Non-ambient, Temp., Press., Temp. & Press.), '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)).

Search  
Example

This screenshot shows the lower portion of the ICDD search interface. The 'Space Group' dropdown menu is open, showing 'P4/mmm' as the selected option. A red arrow points from the 'Select Space Group' text to this dropdown. Other visible filters include 'Crystal System' (Triclinic (Anorthic), Rhombohedral, Monoclinic, Hexagonal, Orthorhombic, Cubic, Tetragonal) and 'Crystal (Symmetry Allowed)' (Centrosymmetric, Non-centrosymmetric). The 'Physical Properties' section includes fields for 'Reduced Cell', 'Author's Unit Cell', and 'Supercell Subcell'. The 'Reference' section has fields for 'a', 'b', 'c' values and errors. The 'Comments' section has a text area.

Select Space  
Group

Selected filters  
highlighted in red

Select Compound Name

This screenshot shows the lower portion of the ICDD search interface. The 'Formula' dropdown menu is open, showing 'Any Formula' as the selected option. A red arrow points from the 'Select Compound Name' text to this dropdown. Other visible filters include 'Name' (Potassium Platinum Chloride), 'IMA No.', 'CAS Number', 'Number of Elements' (Low, High), 'Composition' (Element, Weight %, ± Error), and 'Status' (Primary, Alternate, Deleted). The 'Database' section includes 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'. The 'Physical Properties' section includes 'Reduced Cell', 'Author's Unit Cell', and 'Supercell Subcell'. The 'Reference' section has fields for 'a', 'b', 'c' values and errors. The 'Comments' section has a text area.

# Search Results

Choose fields to be displayed in results

Results - 9 of 412,083

File Fields Tools Help

Open PDF Card Simulated Profile

Search Results

My Defaults

PDF #	QM	Chemical Formula	Compound Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Coords
00-009-0367	I	$K_2 Pt Cl_4$	Potassium Platinum Chloride	6.940000	3.160000	3.550000	T	✓
01-073-1506	I	$K_2 ( Pt Cl_4 )$	Potassium Platinum Chloride	6.990000	3.169250	3.555730	T	✓
04-006-6128	P	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	✓
04-007-2797	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.023000	3.183810	3.571940	T	✓
04-007-5356	I	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.025000	3.182100	3.569270	T	✓
04-007-7303	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	6.996100	3.159080	3.540590	T	✓
04-007-7304	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	6.981300	3.156210	3.538480	T	✓
04-009-8290	B	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	✓
04-013-8855	B	$K_2 Pt ( CN )_4 Cl_{0.32} ( H_2 O )_{2.6}$	Potassium Platinum Chloride Cyanid...	9.866000	4.412210	6.976320	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 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 ICDD Filters, Formula/Name, Classifications, Crystallography, Diffraction, Neutron 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), SYS, and Coords. A red arrow points from the 'Add data fields to selected list' annotation to the right-pointing arrow button between the two lists. Another red arrow points from the 'Order the data fields in the selected list' annotation to the left-pointing arrow button. A third red arrow points from the 'Remove data fields from the selected list' annotation to the 'Reset' button at the bottom left. The 'Include Deleted Patterns' checkbox is unchecked. The bottom right contains 'OK', 'Cancel', 'Apply', and 'Help' buttons.

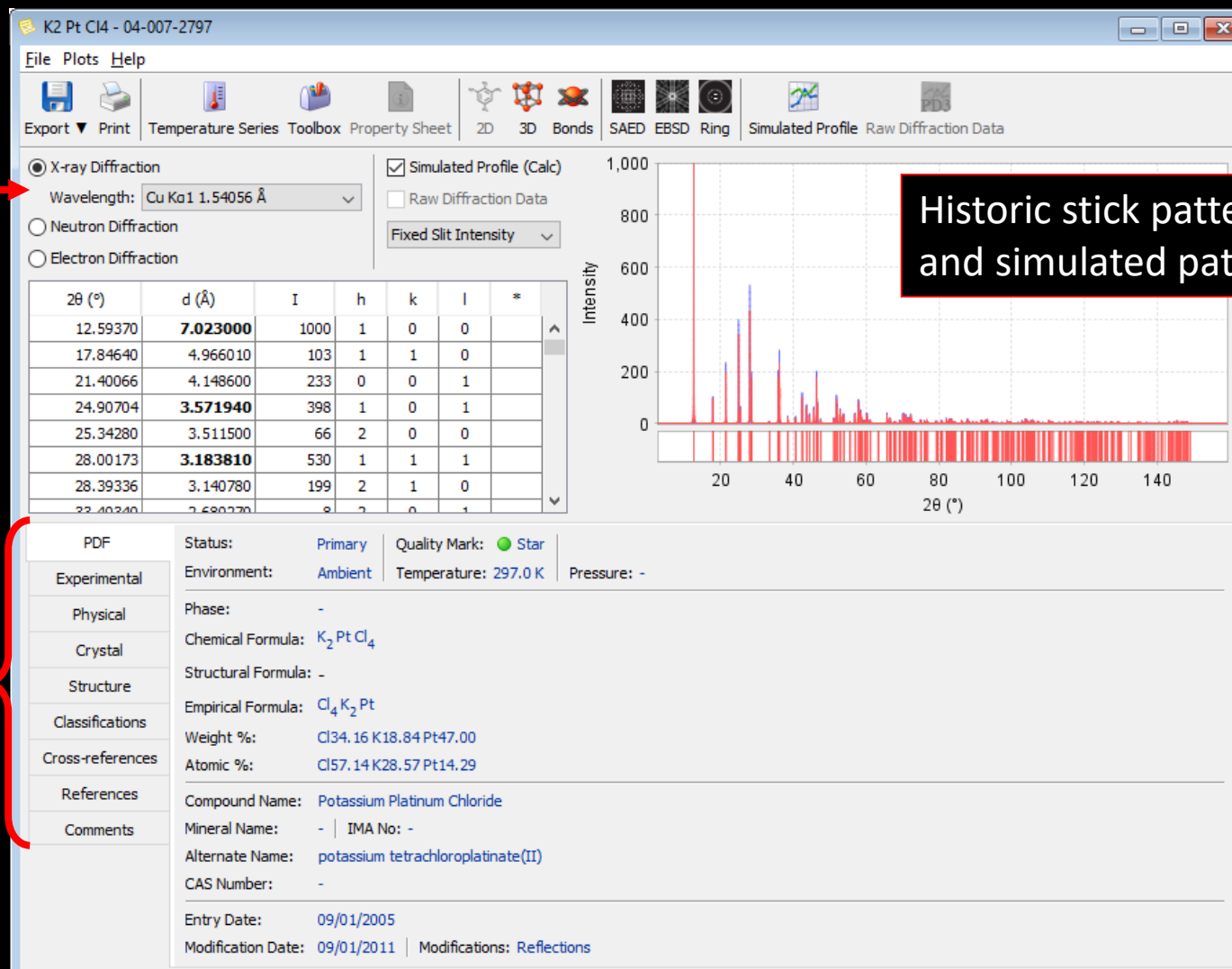
Add data fields to selected list

Order the data fields in the selected list

Remove data fields from the selected list

# PDF Data Card

Choose  
equipment  
factors



Tabular view of reported data



# PDF Data Card

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

Open multiple PDF Cards.

Results - 9 of 412,083

File Fields Tools Help

Open PDF Card Simulated Profile

PDF #	QM	Chemical Formula	
00-009-0367	I	$K_2PtCl_4$	Potassi
01-073-1506	I	$K_2(PtCl_4)$	Potassi
04-006-6128	P	$K_2PtCl_4$	Potassi
04-007-2797	S	$K_2PtCl_4$	Potassi
04-007-5356	I	$K_2PtCl_4$	Potassi
04-007-7303	S		
04-007-7304	S		
04-009-8290	B		
04-013-8855	B		

[[Pt And Cl]] And [Any Name 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 - 04-007-7303

K2 (Pt Cl4) - 01-073-1506

K2 Pt Cl4 - 00-009-0367

Wavelength: Cu K $\alpha$  1.54056 Å

Simulated Profile (Exp-based)

Intensity

2 $\theta$  (°)

PDF

Status: Primary Quality Mark: Indexed

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

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

Modification Date: - Modifications: -

# PDF Data Card Features



## View Temperature Series

Temperature Series (K2 Pt Cl4 - 04-007-2797)

File Fields Set: Temperature Series Tools Help

Temp (K)	PDF #	QM	Chemical Formula	Compound Name	RedCell Vol (Å³)	Author
120.0	04-007-7303	S	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	200.93	Takazawa H., Oh
120.0	04-007-7304	S	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	200.06	Takazawa H., Oh
293.0	04-007-5356	I	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	204.51	Mais R.H.B., Ovi
297.0	04-009-8290	B	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	204.60	Ohba S., Sato
297.0	04-007-2797	S	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	204.62	
298.0	00-001-0103	I	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	201.79	Hanawalt, J. et
298.0	00-009-0367	I	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	201.96	Staritzky, R.
298.0	01-073-1506	I	K <sub>2</sub> (Pt Cl <sub>4</sub> )	Potassium Platinum Chloride	201.79	Dickinson, R.G.
298.0	04-006-6128	P	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	204.60	Ohba S., Matsud

## View Toolbox

Toolbox

Author's Cell Parameters

a (Å): 7.023 b (Å): 7.023 c (Å): 4.1486

α (°): 90 β (°): 90 γ (°): 90

☐ Edit Cell Parameters

Wavelength (Å): 1.540598

Peak Planar Angles Reflections

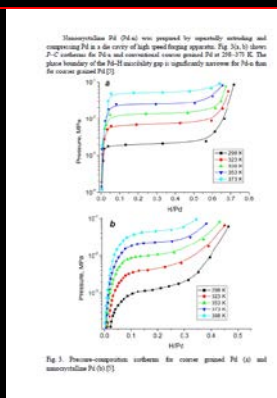
Miller Index Results

h: 0 d: 4.149 Å

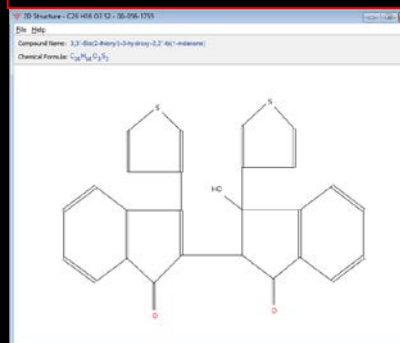
k: 0 2θ: 21.401°

l: 1

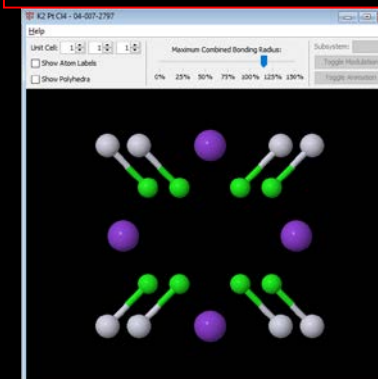
## View Property Sheet



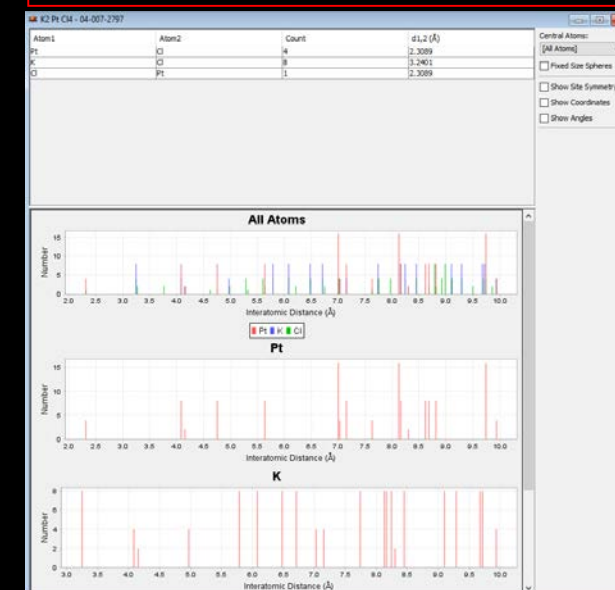
## View 2D Structure



## View 3D Structure



## View Bond Distances/Angles

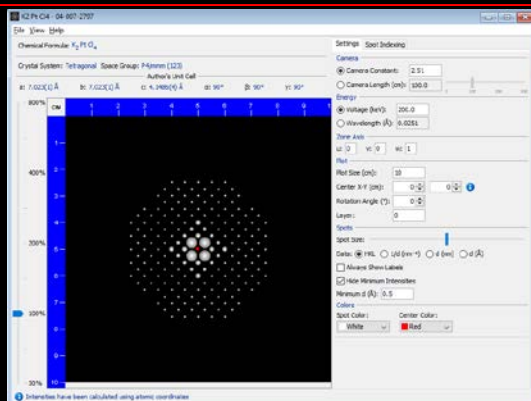


Note: The availability of each feature varies by PDF entry.

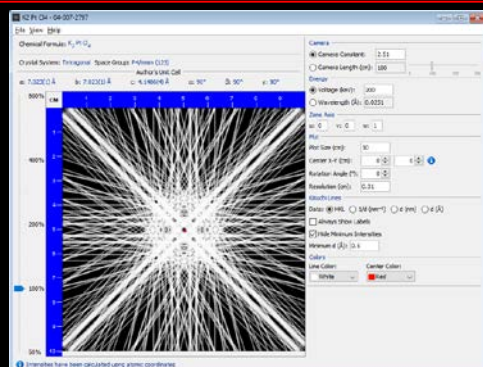
# PDF Data Card Features



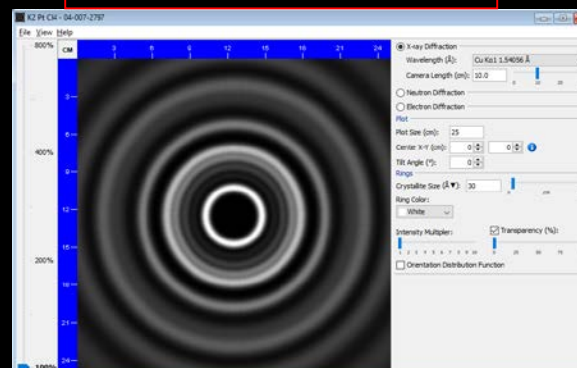
View Simulated Electron Spot Pattern



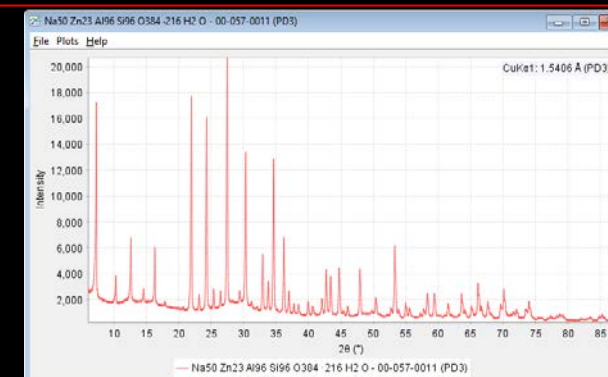
View Electron Backscattering Pattern



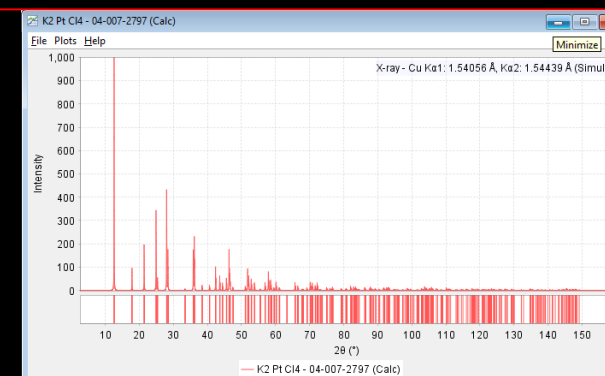
View Ring Pattern



View Raw Diffraction Data (PD3)



View Simulated Diffraction Profile





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