

# PDF-4+ Tools and Searches



# PDF-4+ 2021

The PDF-4+ 2021 database is powered by our integrated search display software. PDF-4+ 2021 boasts 77 search selections coupled with 131 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+ 2021.

PDF-4+ 2021

File Edit Window Help

Open PDF Cards Preferences Search History Results Composition Graph Sieve + 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

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	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.811	6 C 12.01	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
3	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.065	17 Cl 35.453	18 Ar 39.948
4	19 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	37 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	55 Cs 132.905	56 Ba 137.327	57 La 138.908	72 Hf 178.49	73 Ta 180.948	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.967	80 Hg 200.59	81 Tl 204.383	82 Pb 207.2	83 Bi 208.98	84 Po [209]	85 At [210]	86 Rn [222]
7	87 Fr [223]	88 Ra [226]	89 Ac [227]	104 Rf [261]	105 Db [262]	106 Sg [266]	107 Bh [264]	108 Hs [277]	109 Mt [278]	110 Ds [271]	111 Rg [272]	112 Cn [285]	113 Nh [286]	114 Fl [289]	115 Mc [289]	116 Lv [293]	117 Ts [294]	118 Og [294]
La			57 La 138.908	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			89 Ac [227]	90 Th 232.038	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]	

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Range Input

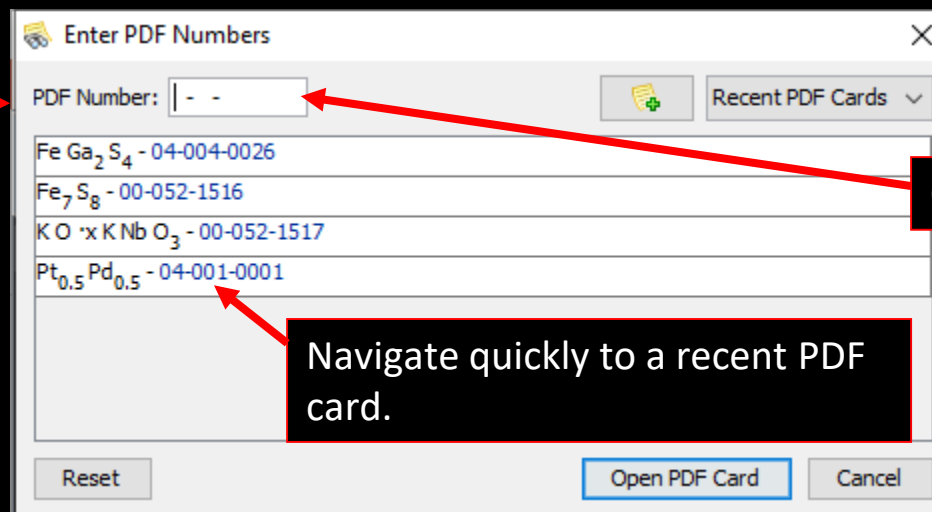
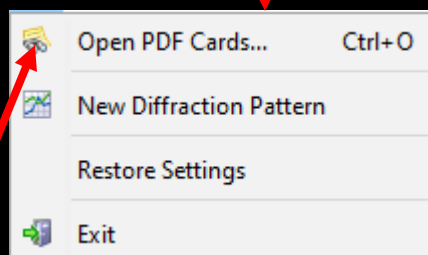
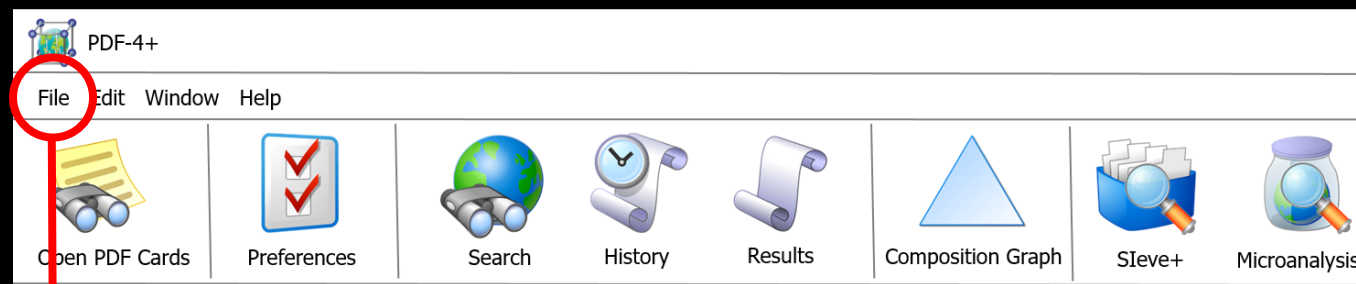
Global Operator

Search Reset Tab Reset All Help

Tool Bar

Primary Search Menu

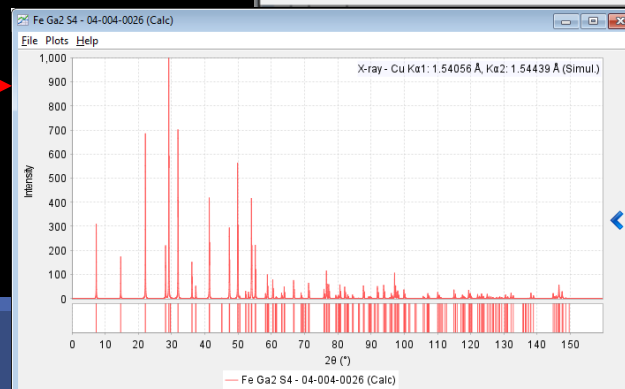
# Getting Started



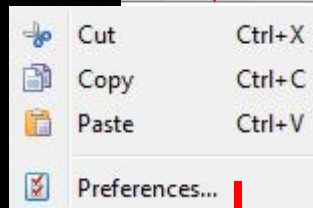
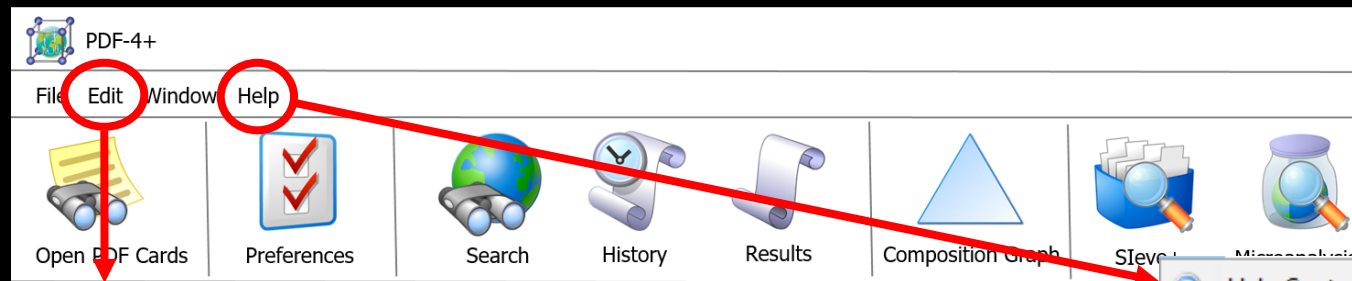
Open a known PDF card.

Navigate quickly to a recent PDF card.

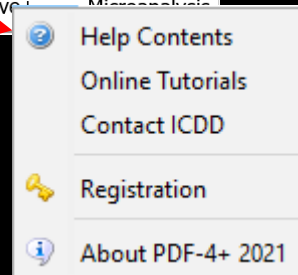
Open a previously saved diffraction pattern. The pattern must be of the ICDD XML file format. All PDF entries can be saved in this format.



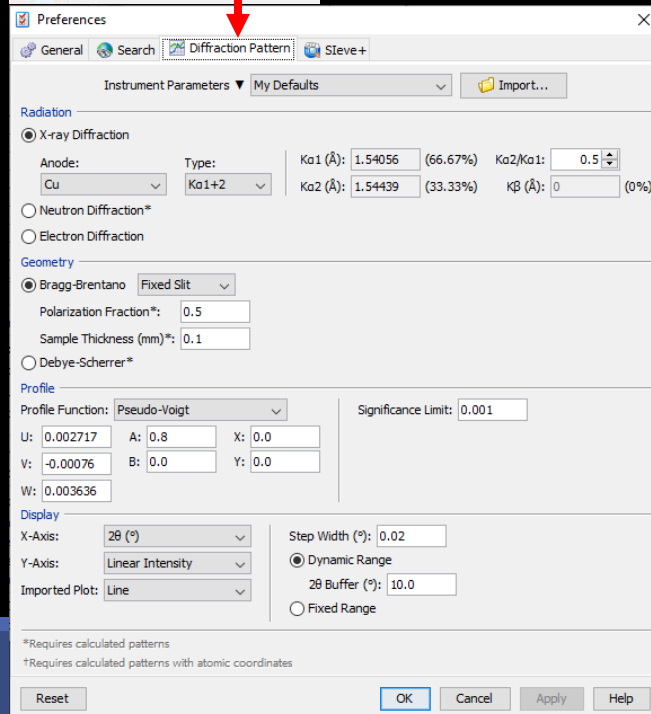
# Getting Started



Edit functions

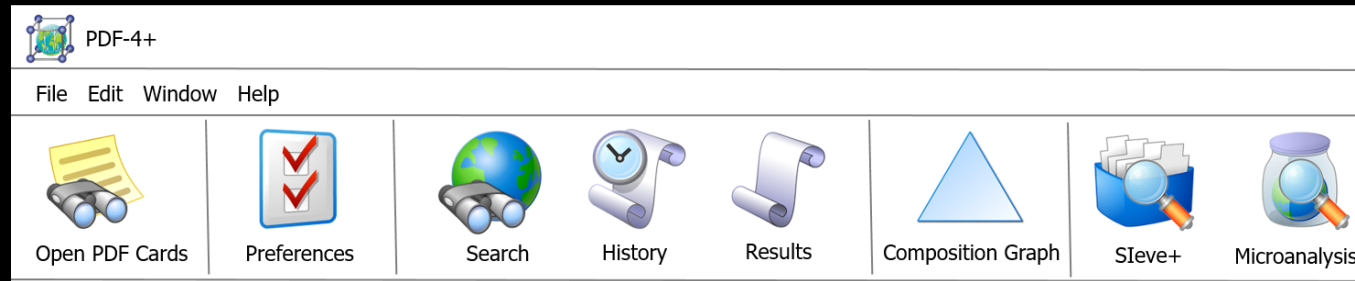


Help information regarding use, support, license policy, and registration of the PDF-4+.



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



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-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.

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

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial.
- Environment:** Ambient, 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.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).

Below the search criteria is a periodic table with columns 1 through 18. The table includes elements from Hydrogen (H) to Oganesson (Og). The interface also features a 'Range Input' and 'Global Operator' section at the bottom.

Periodic Table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Formula/Name	1 H 1.008																	2 He 4.003
Classifications	3 Li 6.941	4 Be 9.012											5 B 10.811	6 C 12.01	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
Crystallography	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.065	17 Cl 35.453	18 Ar 39.948
Modulated	19 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
Diffraction	37 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 131.29
Physical Properties	55 Cs 132.905	56 Ba 137.327	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	
Reference	73 Ta 180.948	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.22	78 Pt 195.078	79 Au 196.967	80 Hg 200.59	81 Tl 204.383	82 Pb 207.2	83 Bi 208.98	84 Po [209]	85 At [210]	86 Rn [222]				
Comments	87 Fr [223]	88 Ra [226]	89 Ac [227]	90 Th 232.038	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]	

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

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

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

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

1 H 1.008

2 Li 6.941 Be 9.012

3 Na 22.990 Mg 24.305

4 K 39.098 Ca 40.078 Sc 44.956 Ti 47.867 V 50.941 Cr 51.998 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

6 Cs 132.905 Ba 137.327 Hf 178.49 Ta 180.948 W 183.84

7 Fr 223 Ra 226 Rf 261 Db 262 Sg 266

La 138.906 Ce 140.116 Pr 140.908 Nd 144.242

Ac 227 Th 232.038 Pa 231.036 U 238.029

Boolean ☐ Yes/No/Maybe ☐ Composition List

And ☐ Or ☐ Not Grouping: ☐ And ☐ Or

Only ☐ Just

Range Input ▼

Global Operator ▼

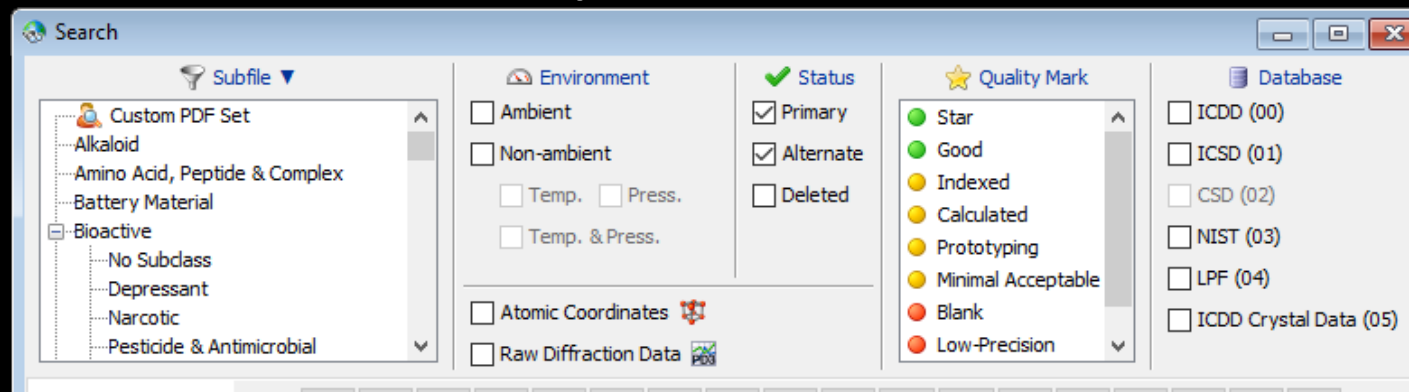
Search Reset Tab Reset All Help

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

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

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

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

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 51.998 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 102.905 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 131.29

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 190.23 77 Ir 192.217 78 Pt 195.078 79 Au 196.967 80 Hg 200.59 81 Tl 204.383 82 Pb 207.2 83 Bi 208.98 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 272 112 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 227 89 Ac 227 90 Th 232.038 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

Range Input ▼

Global Operator ▼

Search Reset Tab Reset All Help

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 a periodic table.

**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

**Database:**

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

**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' is selected under the 'Select 2-5 elements' dropdown. The search results are displayed on the right, showing a list of empirical formulas and their corresponding hits.

Empirical Formula	Hits
Fe	129
Fe <sub>0.95</sub> Ni <sub>0.05</sub>	4
Fe <sub>0.9463</sub> Ni <sub>0.0537</sub>	1
Fe <sub>0.946</sub> Ni <sub>0.054</sub>	1
Fe <sub>0.9458</sub> Ni <sub>0.0542</sub>	1
Fe <sub>0.9441</sub> Ni <sub>0.0559</sub>	1
Fe <sub>0.9429</sub> Ni <sub>0.0571</sub>	1
Fe <sub>0.94</sub> Ni <sub>0.06</sub>	2
Fe <sub>0.9381</sub> Ni <sub>0.0619</sub>	1
Fe <sub>0.92</sub> Ni <sub>0.08</sub>	1
Fe <sub>0.916</sub> Ni <sub>0.084</sub>	24
Fe <sub>10.8</sub> Ni	1
Fe <sub>0.91</sub> Ni <sub>0.09</sub>	2
Fe <sub>0.9</sub> Ni <sub>0.1</sub>	3

# Search Window

## Formula/Name

The screenshot shows the 'Search' window with various filter categories on the left and search criteria on the right. A red arrow points from the 'Any Formula' option in the left sidebar to the 'Formula' dropdown menu in the search criteria section.

**Search Window Interface:**

- 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.
- Search Criteria:** Formula (dropdown), Name, IMA No., CAS No., Number of Elements (Low, High), Molecular Wt (g/mol) (Value, ±Error), Composition (Element, Weight %, ±Error).
- Left Sidebar:** Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, Comments.

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.

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

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

**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

The screenshot shows the ICDD Search Window interface. The top section contains several filter categories: Subfile, Environment, Status, Quality Mark, and Database. The Subfile list includes Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial. The Environment section has checkboxes for Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, and Raw Diffraction Data. The Status section has checkboxes for Primary, Alternate, and Deleted. The Quality Mark section has a list of quality levels: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision. The Database section has checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05). The bottom section contains a search bar and a list of search criteria: Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The Formula/Name section is expanded, showing a search bar and a dropdown menu for Name. The Name dropdown menu is open, showing options: Any Name, Compound Name, Mineral Name, Alternate Name, Zeolite Name, Contains Fragments, Contains Phrase, Exactly, and Not. A red arrow points from the 'Name' dropdown menu to the 'Any Name' option.

Search Window

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

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

Formula

Any Formula

Name

Any Name

IMA No.

Number of Elements

Low High

Molecular Wt (g/mol)

Value ±Error

Composition

Element Weight

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.

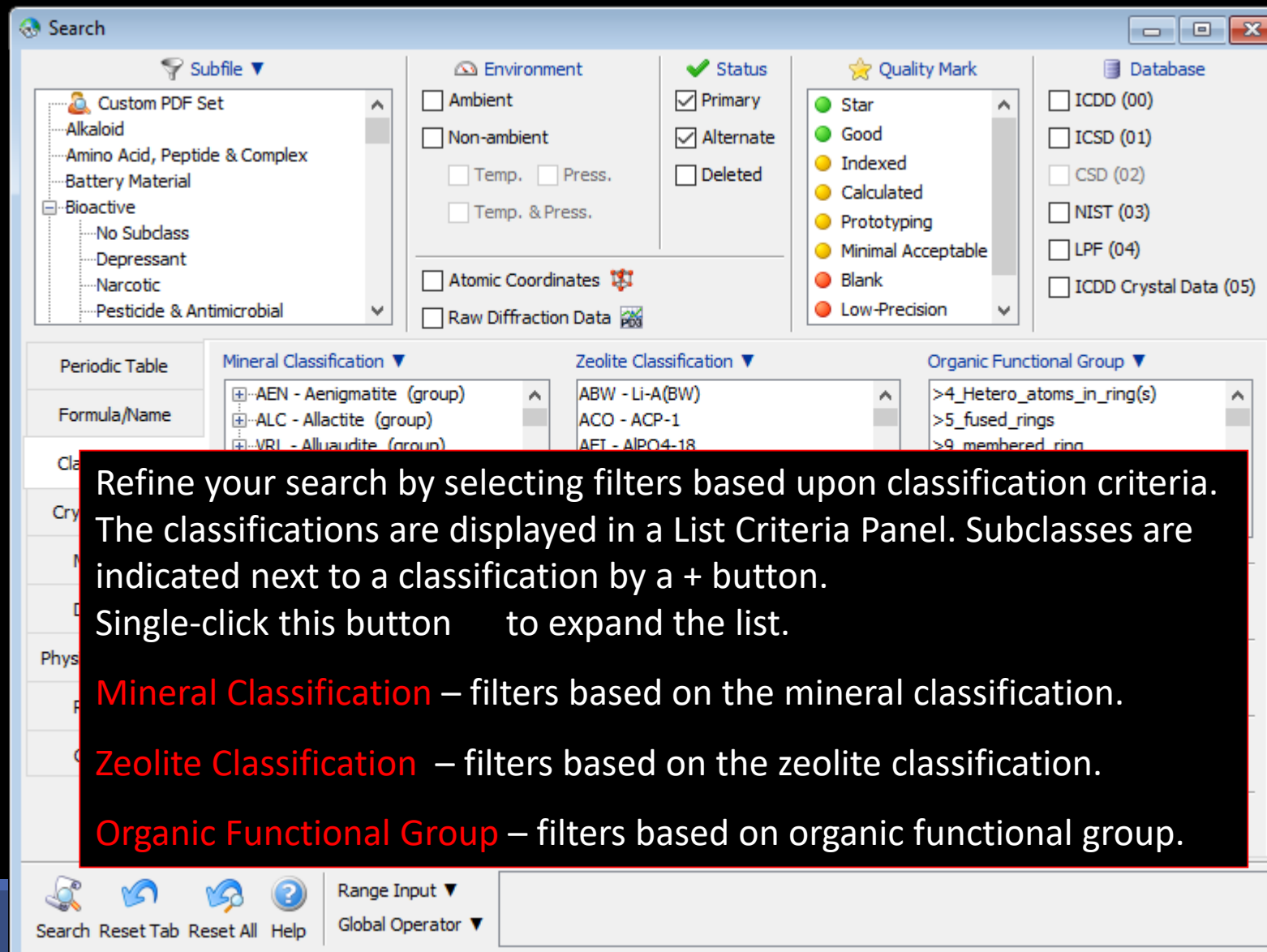
**Alternate Name** – filters based on another recognized name of the material.

**Zeolite Name** – filters based on the zeolite name.



# Search Window

## Classifications



The screenshot displays the 'Search' window with several filter panels. The 'Subfile' panel on the left lists categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The 'Environment' panel includes checkboxes for 'Ambient', 'Non-ambient', 'Temp.', 'Press.', and 'Temp. & Press.'. The 'Status' panel has checkboxes for 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' panel features a list of quality levels: 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', 'Minimal Acceptable', 'Blank', and 'Low-Precision'. The 'Database' panel lists 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'. Below these, three classification panels are visible: 'Mineral Classification' (listing 'AEN - Aenigmatite (group)', 'ALC - Allactite (group)', and 'VRI - Alluaudite (group)'), 'Zeolite Classification' (listing 'ABW - Li-A(BW)', 'ACO - ACP-1', and 'AET - AIPO4-18'), and 'Organic Functional Group' (listing '>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 use the classification 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 'Search' window with various filter tabs. The 'Pearson Symbol' filter is selected, showing a dropdown menu with 'With Hydrogen' and 'Without Hydrogen' options. A red arrow points to this dropdown with the annotation: 'Filters for Pearson Symbol Codes with and without Hydrogen.' Below it, the 'Prototype Structure' filter is shown with a dropdown menu set to 'Any Prototype Structure'. A red arrow points to this dropdown with the annotation: 'Filters based on a user-constructed Pearson Symbol Code.'

**Search Window Interface:**

- 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.
- 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).
- Zeolite Classification:** ABW - Li-A(BW), ACO - ACP-1, AEI - AIPO4-18, AEL - AIPO4-11, AEN - AIPO-EN3.
- 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 (selected).
- Prototype Structure:** Any Prototype Structure.
- Formula Type (ANX):**
- Wyckoff Sequence:**
- Range Input:**
- Global Operator:**
- Search Buttons:** Search, Reset Tab, Reset All, Help.



# Search Window

## Crystallography

The screenshot shows the 'Search' window with the 'Crystallography' tab selected. The window is divided into several sections: 'Subfile' (a tree view of categories like Alkaloid, Amino Acid, etc.), 'Environment' (checkboxes for Ambient, Non-ambient, Temp., Press., etc.), 'Status' (checkboxes for Primary, Alternate, Deleted), 'Quality Mark' (radio buttons for Star, Good, Indexed, etc.), and 'Database' (checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05)). Below these are sections for 'Crystal System' (Triclinic, Monoclinic, Orthorhombic, Tetragonal, Rhombohedral, Hexagonal, Cubic), 'Crystal (Symmetry Allowed)' (Centrosymmetric, Non-centrosymmetric, Enantiomorphic, Pyro / Piezo (p), Optical Activity, Piezo (2nd Harm.)), 'Space Group' (with a 'Space Group Symbol' field), and 'AET' (with 'AET' and 'Elements' fields). At the bottom, there are four tabs: 'Crystal Data', 'Reduced Cell', 'Author's Unit Cell', and 'Supercell/Subcell'. The 'Crystal Data' tab is highlighted with a red oval. A red box contains text explaining these tabs.

Search Window Crystallography

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

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

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

AET

AET

Elements

Value

±Error

Value

±Error

Value

±Error

Search Reset Tab Reset All Help Global Operator

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

# Search Window

## Crystal Data

**Search**

**Subfile**

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

**Environment**

- ☐ Ambient
- ☐ 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

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

**Crystal (Symmetry Allowed)**

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

**Space Group**

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

**AET**

AET  ...

Elements

**Unit Cell**

Value  ±Error

**Volume**

Value  ±Error

**Axial Ratio**

c/a: Value  ±Error

a/b: Value  ±Error

c/b: Value  ±Error

**Search** **Reset Tab** **Reset All** **Help** **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

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

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

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume

Value ±Error

Axial Ratio

c/a: Value ±Error

c/b: Value ±Error

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

Filters based on the volume of the crystal data.

Range Input ▼

Global Operator ▼

Search Reset Tab Reset All Help

ISO 9001:2015  
QUALITY MANAGEMENT SYSTEM CERTIFIED  
BY DEKRA  
CERT. NO.  
110409.01

# 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

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

Volume

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.

Range Input ▼

Global Operator ▼

Search Reset Tab Reset All Help

ICDD<sup>®</sup>  
INTERNATIONAL CENTER FOR DIFFRACTION DATA

ISO 9001:2015  
QUALITY MANAGEMENT SYSTEM CERTIFIED  
BY DEKRA  
CERT. NO. 110409.01

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

Filters based on the volume of the reduced cell.

# Search Window

## Author's Cell

The screenshot shows the ICDD Search Window with the 'Author's Cell' tab selected. The window is divided into several sections: Subfile, Environment, Status, Quality Mark, and Database. The 'Author's Cell' section contains input fields for Crystal Data, Reduced Cell, and Supercell/Subcell. A 'Convert Cell' dialog box is open, showing options to convert from Triclinic (Anorthic) to either Crystal Data or Reduced Cell. Red arrows and text boxes provide additional context:

- Convert Cell form used to convert Author's Unit Cell Axis/Volume data to Crystal or Reduced Cell Axis/Volume data for searching.** (Points to the 'Convert Cell' dialog box)
- Filters based on the lengths of the three axes of the author's cell.** (Points to the 'Axis (Å)' section in the 'Author's Cell' tab)
- Filters based on the volume of the author's unit cell.** (Points to the 'Volume' section in the 'Author's Cell' tab)

The 'Author's Cell' section includes the following input fields:

Axis (Å)		Volume		Axial Ratio	
a:	Value ±Error	a:	Value ±Error	c/a:	Value ±Error
b:	Value ±Error	β:	Value ±Error	a/b:	Value ±Error
c:	Value ±Error	γ:	Value ±Error	c/b:	Value ±Error

The 'Convert Cell' dialog box shows the following options:

- Crystal System: Triclinic (Anorthic)
- Bravais Lattice: Primitive
- ☒ Convert to Crystal Data
- ☐ Convert to Reduced Cell

The bottom of the window features a 'Range Input' section with 'Search', 'Reset Tab', 'Reset All', and 'Help' buttons, and a 'Global Operator' dropdown.

# Search Window

## Supercell/Subcell

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

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

- Subfile:** Custom PDF Set, Alkaloid, Complex, Microbial.
- 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.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).
- 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.).
- AET:** AET, Elements.
- Space Group:** Space Group Symbol.
- Crystal Data:** Reduced Cell, Author's Unit Cell, **Supercell/Subcell** (selected).
- Axis (Å):** a, b, c, α, β, γ, with Value and ±Error fields.
- Supercell/Subcell:** Supercell (selected), Subcell, Volume Ratio: 1 to 1.
- Bottom Bar:** 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

Environment

☐ Ambient

☐ Non-ambient

☐ Temp. ☐ Press.

☐ Temp. & Press.

☐ Atomic Coordinates

☐ Raw Diffraction Data

Status

☒ Primary

☒ Alternate

☐ Deleted

Quality Mark

☒ Star

☐ Minimal Acceptable

☐ Blank

☐ Low-Precision

Database

☐ ICDD (00)

☐ LPF (04)

☐ 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 Subsystem)

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

The screenshot shows the 'Search' window for Diffraction data. The interface is divided into several sections:

- Subfile:** A tree view on the left 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:** A list of quality marks with corresponding colored circles: Star (green), Good (green), Indexed (yellow), Calculated (yellow), Prototyping (yellow), Minimal Acceptable (yellow), Blank (red), and Low-Precision (red).
- Database:** Checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'.
- Search Criteria:** A central area with various filters:
  - Periodic Table:** A dropdown menu.
  - Formula/Name:** Input fields for 'Value' and '±Error'.
  - Classifications:** Checkboxes for 'D1', 'D2', and 'D3'.
  - Crystallography:** Checkboxes for 'Integrated Intensities' and 'Peak Intensities'.
  - Modulated:** A checkbox.
  - Diffraction:** A dropdown menu for 'I/I-corundum' with 'Value' and '±Error' input fields.
  - Physical Properties:** A dropdown menu for 'R-factor' with 'Value' and '±Error' input fields.
  - Reference:** A dropdown menu for 'Temperature of Data Collection (K)' with 'Value' and '±Error' input fields.
  - Comments:** A dropdown menu for 'Smith-Snyder Figure of Merit' with 'Value' and '±Error' input fields.
  - Temperature of Data Collection (K):** Input fields for 'Value' and '±Error'.
  - Pressure of Data Collection (GPa):** Input fields for 'Value' and '±Error'.
- Bottom Bar:** Includes a 'Range Input' dropdown, a 'Global Operator' dropdown, and buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help'.

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

The screenshot shows the 'Physical Properties' section of the ICDD Search Window. On the left is a vertical sidebar with categories: Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties (selected), Reference, and Comments. The main area contains filters for Melting Point (K), Density (g/cm³), Color, and Topology. The Melting Point filter has a dropdown menu open showing options: Kelvin (K), Celsius (°C), Fahrenheit (°F), and Not. The Density filter has checkboxes for Measured Density, Calculated Density, and Structural Density. The Color filter has a list of color options. The Topology filter has a text input field. At the bottom are buttons for Search, Reset Tab, Reset All, and Help, along with Range Input and Global Operator dropdowns.

Search Window

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

Database

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

Physical Properties

Melting Point (K) ▼

Value  ±Error

Density (g/cm³) ▼

Value  ±Error

☒ Measured Density ☒ Calculated Density ☒ Structural Density

Color ▼

- Black
- Blue
- Brown
- Color Missing
- Colorless
- Gray

☐ Property Sheet ☐ Topology Data

Topology ▼

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

Environment

☐ Ambient

☐ Non-ambient

☐ Temp. ☐ Press.

☐ Temp. & Press.

☐ Atomic Coordinates

☐ Raw Diffraction Data

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Search All Re

Author ▼

Title ▼

Publication ▼

Journal/Patent

Year

Start Year

End Year

DOI

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


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

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:

Filter based on the text contained in comments.

Search Reset Tab Reset All Help

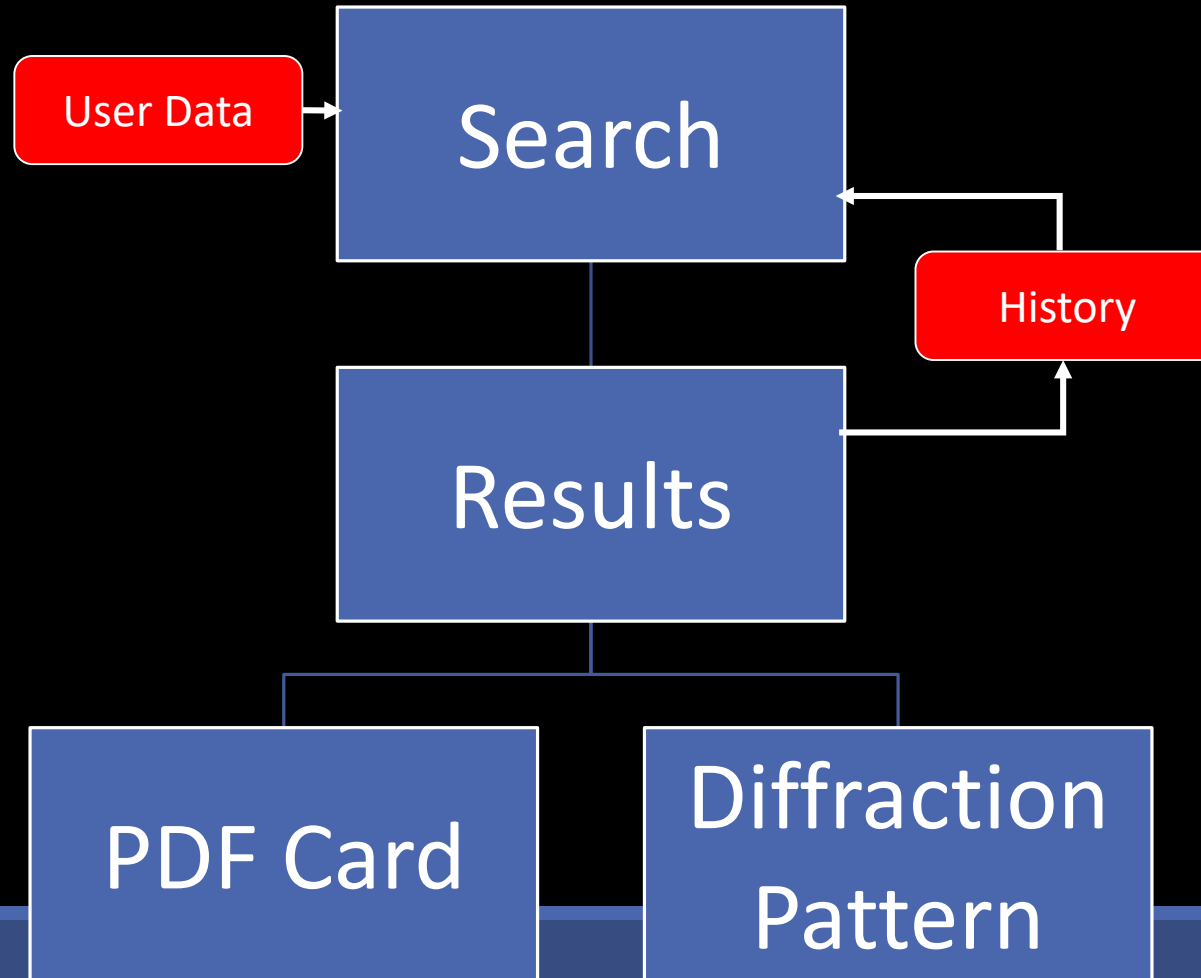
Range Input ▼

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.



Select  
Elements in  
Periodic Table

# Search Example

The screenshot displays the ICDD search interface with several filters highlighted in red boxes and arrows:

- Select Elements in Periodic Table:** A red box highlights the 'Periodic Table' section, with an arrow pointing to the 'Pt And Cl' selection in the 'Classifications' list.
- Select Space Group:** A red box highlights the 'Space Group' dropdown menu, which is set to 'P4/mmm'.
- Select Compound Name:** A red box highlights the 'Name' dropdown menu, which is set to 'Potassium Platinum Chloride'.
- Selected filters highlighted in red:** A red box highlights the 'Status' section, which includes 'Primary', 'Alternate', and 'Deleted' filters.

The search results at the bottom show the following query: `[[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

Choose fields to be displayed in results

Results - 9 of 444,133

File Fields Tools Help

Open PDF Card Simulated Profile

Search Results My Defaults

PDF #	I/Ic	QM	Chemical Formula	Compound Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Temp (K)	Coords
00-009-0367		● I	$K_2PtCl_4$	Potassium Platinum Chloride	6.940	3.160	3.550	T	298.0	✓
01-073-1506	8.65	● I	$K_2(PtCl_4)$	Potassium Platinum Chloride	6.990000	3.169250	3.555730	T	298.0	✓
04-006-6128	8.86	● P	$K_2PtCl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	298.0	✓
04-007-2797	8.79	● S	$K_2PtCl_4$	Potassium Platinum Chloride	7.023000	3.183810	3.571940	T	297.0	✓
04-007-5356	8.8	● I	$K_2PtCl_4$	Potassium Platinum Chloride	7.025000	3.182100	3.569270	T	293.0	✓
04-007-7303	8.85	● S	$K_2PtCl_4$	Potassium Platinum Chloride	6.996100	3.159080	3.540590	T	120.0	✓
04-007-7304	8.84	● S	$K_2PtCl_4$	Potassium Platinum Chloride	6.981300	3.156210	3.538480	T	120.0	✓
04-009-8290	8.77	● B	$K_2PtCl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	297.0	✓
04-013-8855	9.02	● B	$K_2Pt(CN)_4Cl_{0.32}(H_2O)_{2.6}$	Potassium Platinum Chloride Cyanide Hydrate	9.866000	4.412210	6.976320	T	298.0	✓

[(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 folders for ICDD Filters, Formula/Name, Classifications, Crystallography, Diffraction, Neutron Diffraction, Physical Properties, Reference, and Comments. The 'Selected Fields' list on the right contains: PDF #, I/Ic, QM, Chemical Formula, Compound Name, D1 (Å), D2 (Å), D3 (Å), SYS, Temp (K), 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.

Add data fields to selected list

Order the data fields in the selected list

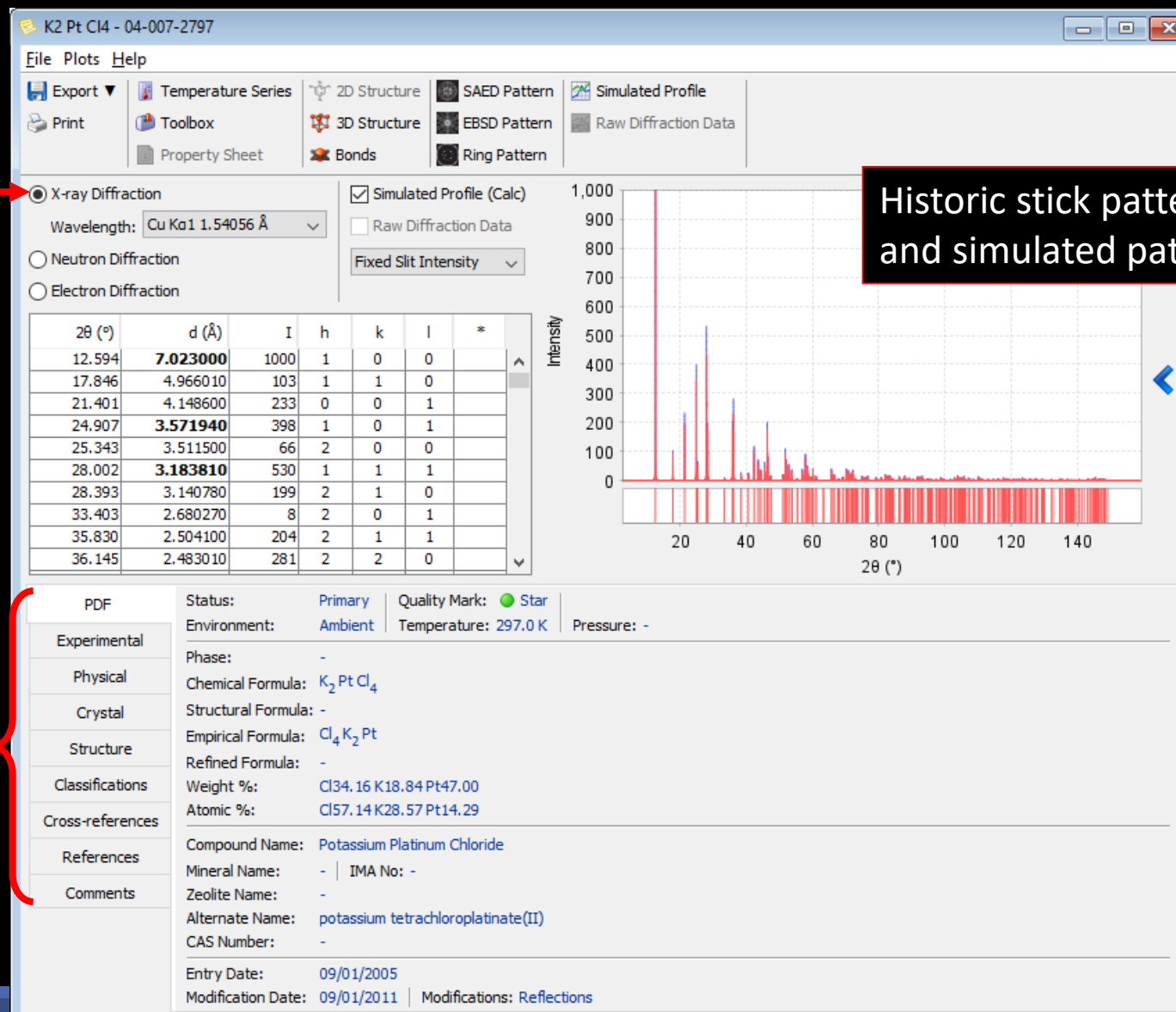
Remove data fields from the selected list

# PDF Data Card

Choose equipment factors

Historic stick pattern and simulated pattern

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 444,133

File Fields Tools Help

Open PDF Card Simulated Profile

PDF #	I/Ic	QM	Chemical Formula	Compound Name
00-009-0367		I	$K_2PtCl_4$	Potassium Platinum
01-073-1506	8.65	I	$K_2(PtCl_4)$	Potassium Platinum
04-006-6128	8.86	P	$K_2PtCl_4$	Potassium Platinum
04-007-2797	8.79	S	$K_2PtCl_4$	Potassium Platinum
04-007-5356	8.8	I	$K_2PtCl_4$	Potassium Platinum
04-007-7303	8.85	S	$K_2PtCl_4$	Potassium Platinum
04-007-7304	8.84	S	$K_2PtCl_4$	Potassium Platinum
04-009-8290	8.77	B	$K_2PtCl_4$	Potassium Platinum
04-013-8855	9.02	B	$K_2PtCl_4$	Potassium Platinum

[[Pt And Cl]] And [Any Name Contain Alternate]]

- Open PDF Card
- Tools/Simulations
- Add to Custom PDF Set...
- Remove from Custom PDF Set...
- Copy Chemical Formula
- Remove Rows

K2 Pt Cl4 - 04-007-7303

File Plots Help

Export Print

Wavelength: Cu Kα1

X-ray Diffraction

Wavelength: Cu Kα1

Simulated Profile (Exp-based)

Wavelength: Cu Kα1 1.54056 Å

Fixed Slit Intensity

Intensity

2θ (°)

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:  $Cl_4K_2Pt$

Refined Formula: -

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: -

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)

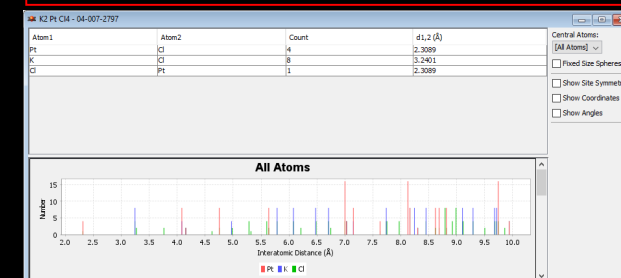
File Fields Set: Temperature Series Tools Help

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

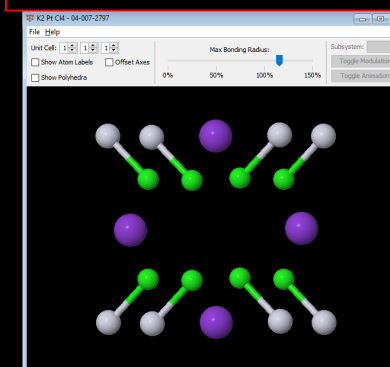
Temperature Series (K2 Pt Cl4 - 04-007-2797)

Temp (K)	PDF #	QM	Chemical Formula	Compound Name	RedCell Vol (Å³)	Author
298.0	04-006-6128	P	K <sub>2</sub> Pt Cl <sub>4</sub>	Potassium Platinum Chloride	204.60	Ohba S., Matsuda T., Harada J., J. Ph

View Bond Distances/Angles



View 3D Structure



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

View Toolbox

Settings

Wavelength: Cu Kα1 1.54056 Å

a (Å): 7.023 a (°): 90  
 b (Å): 7.023 β (°): 90  
 c (Å): 4.1486 γ (°): 90

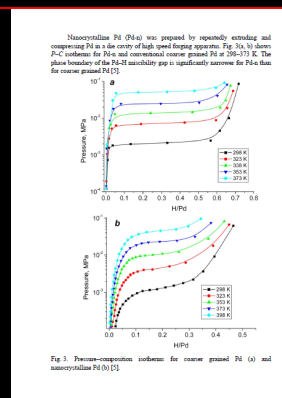
Calculate Peak

h: ☐ k: ☐ l: ☐ 2θ: ☐  
 d-spacing: ☐ Angle: ☐

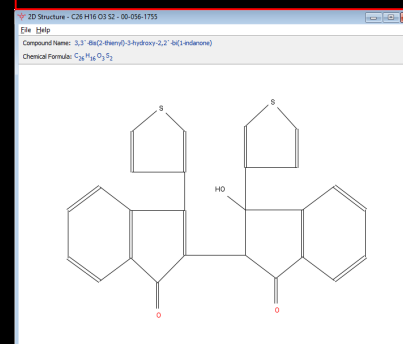
Calculate Peak List

Start 2θ (°):   
 Stop 2θ (°):

View Property Sheet



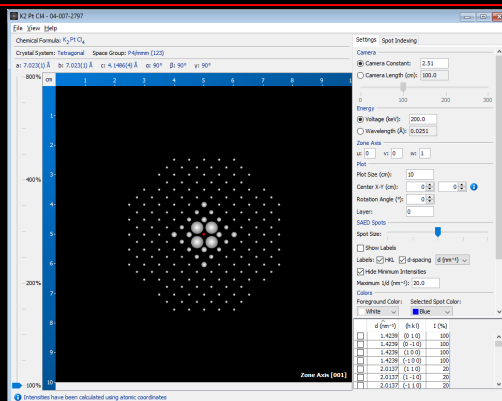
View 2D Structure



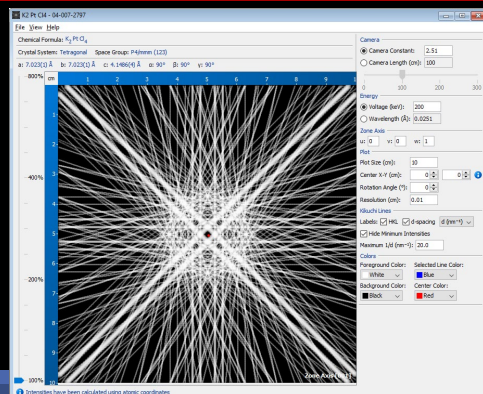
# PDF Data Card Features



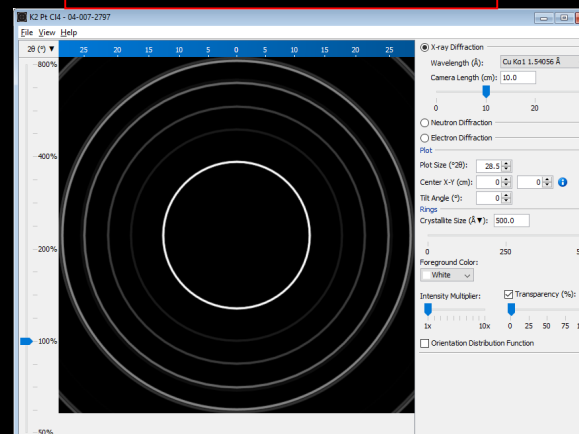
View Simulated Electron Spot Pattern



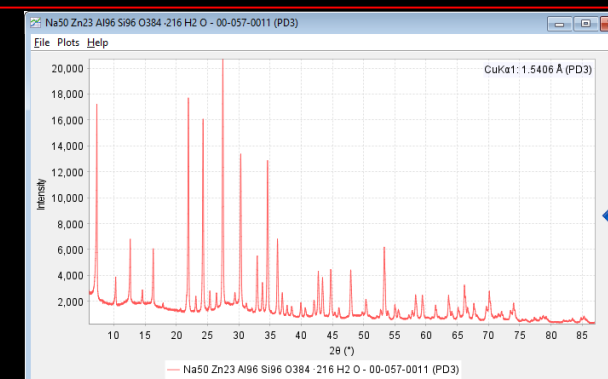
View Electron Backscattering Pattern



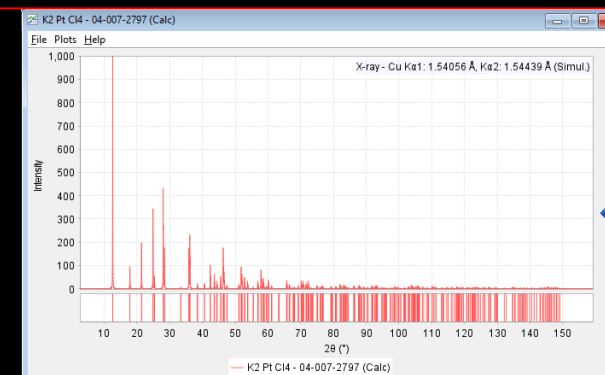
View Ring Pattern



View Raw Diffraction Data (PD3)



View Simulated Diffraction Profile





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

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