

PDF-4+ Tools and Searches



PDF-4+ 2022

The PDF-4+ 2022 database is powered by our integrated search display software. PDF-4+ 2022 boasts 80 search selections coupled with 134 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+ 2022.

PDF-4+ 2022
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
- ☐ 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		
Formula/Name	1 H		Boolean <input checked="" type="radio"/> Yes/No/Maybe <input type="radio"/> Composition List														2 He			
Classifications	3 Li	4 Be	Switch to No											5 B	6 C	7 N	8 O	9 F	10 Ne	
Crystallography	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
Modulated	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr		
Diffraction	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe		
Physical Properties	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn		
Reference	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og		
Comments	La		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
	Ac		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

Range Input
Global Operator

Search Reset Tab Reset All

Tool Bar

Primary Search Menu

Getting Started

The screenshot shows the PDF-4+ 2022 software interface. The 'Open PDF Cards' button in the top toolbar is circled in red. An arrow points from this button to the 'Enter PDF Numbers' dialog box. The dialog box contains a list of PDF cards with their chemical formulas and names. A red arrow points to the 'Recent PDF Cards' dropdown menu, and another red arrow points to the 'Open PDF Card' button at the bottom of the dialog box. Two callout boxes provide instructions: 'Open a known PDF card.' and 'Navigate quickly to a recent PDF card.'

PDF-4+ 2022

File Edit Window Help

Open PDF Cards Preferences Search History Results Composition Graph Sieve+ Microanalysis

Enter PDF Numbers

PDF Number: - - Recent PDF Cards

$((C_6H_7O_2)(C_2H_3O_2)_3)_n$
Cellulose triacetate I
00-064-1453

$ZrH_2P_2O_8 \cdot H_2O$
Zirconium Hydrogen Phosphate Hydrate
00-071-0090

$C_{26}H_{27}F_3N_2O_6$
Tezacaftor
00-071-1635

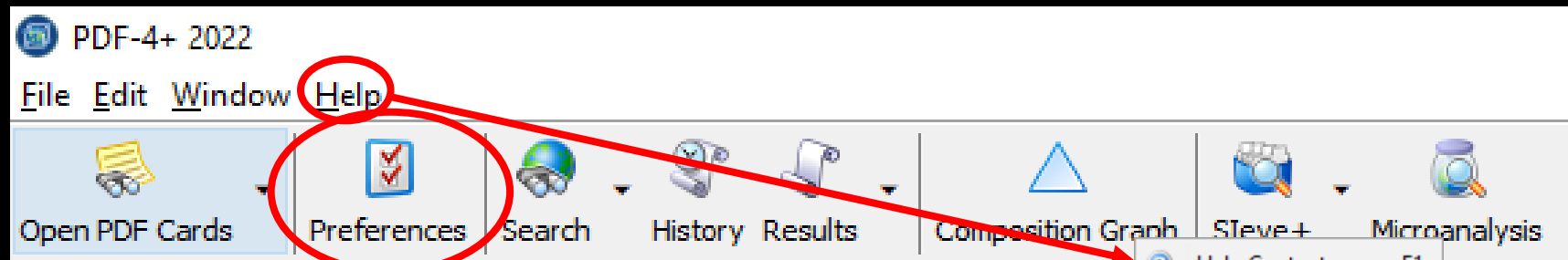
Ca_3SiO_5
Calcium Silicate

Reset Open PDF Card Cancel

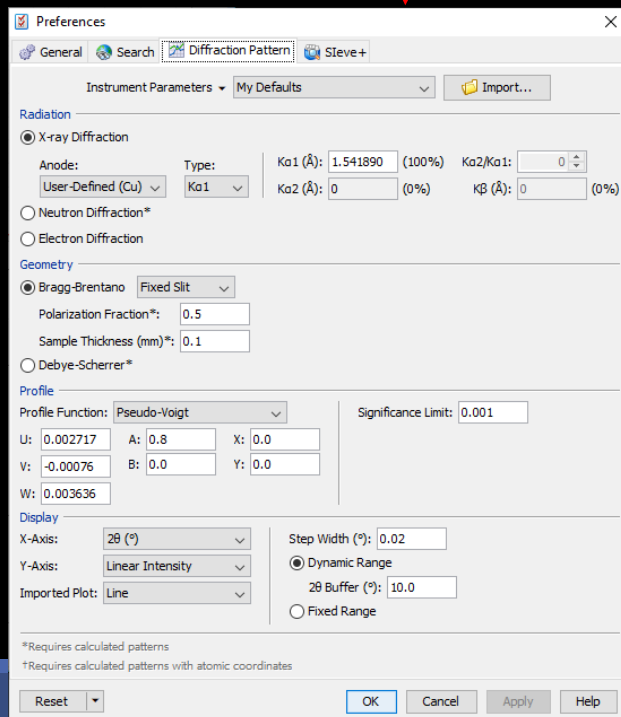
Open a known PDF card.

Navigate quickly to a recent PDF card.

Getting Started

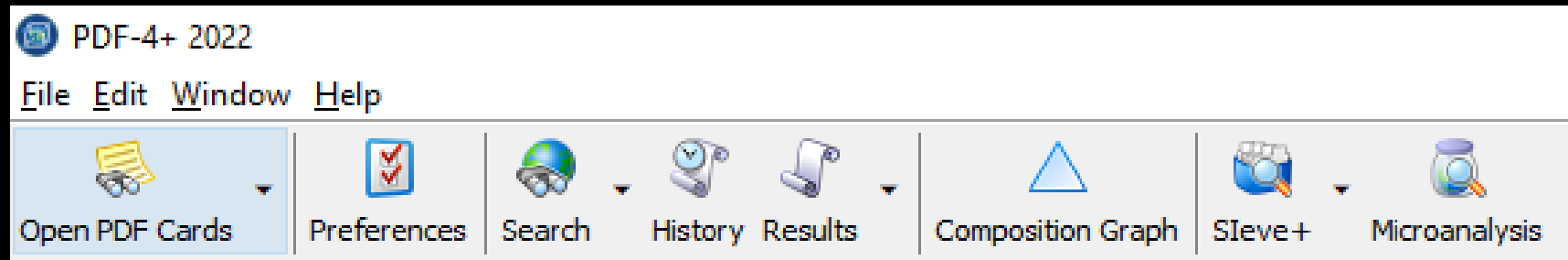


Customize Radiation, Geometry, Profile, Display settings and many more features of the PDF-4+.



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

Tool Bar



Quick Navigation Icons



Open a PDF Card



Select Preferences Module



Open Search Window



Open History Window



Open Results Window



Composition Graph



Open Sieve+



Microanalysis

Primary Search Menu

The Search Window displays nine tabs. Each tab features multiple search criteria to allow you to data mine the PDF-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:** A tree view showing categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'.
- Environment:** Checkboxes for 'Ambient', 'Non-ambient', 'Temp.', 'Press.', 'Temp. & Press.', 'Atomic Coordinates', and 'Raw Diffraction Data'.
- Status:** Checkboxes for 'Primary', 'Alternate', and 'Deleted'.
- Quality Mark:** Radio buttons for 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', 'Minimal Acceptable', 'Blank', 'Low-Precision', and 'Hypothetical'.
- Database:** Checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'.
- Periodic Table:** A table with columns 1-18 and rows 1-7. Elements are color-coded: H (green), He (red), Li (yellow), Be (blue), B (pink), C (green), N (green), O (green), F (yellow), Ne (red), Na (yellow), Mg (blue), Al (pink), Si (pink), P (green), S (green), Cl (yellow), Ar (green), K (yellow), Ca (blue), Sc (light blue), Ti (light blue), V (light blue), Cr (light blue), Mn (light blue), Fe (light blue), Co (light blue), Ni (light blue), Cu (light blue), Zn (light blue), Ga (pink), Ge (pink), As (green), Se (green), Br (yellow), Kr (pink), Rb (yellow), Sr (blue), Y (light blue), Zr (light blue), Nb (light blue), Mo (light blue), Tc (light blue), Ru (light blue), Rh (light blue), Pd (light blue), Ag (light blue), Cd (light blue), In (pink), Sn (pink), Sb (pink), Te (pink), I (yellow), Xe (pink), Cs (yellow), Ba (blue), Hf (light blue), Ta (light blue), W (light blue), Re (light blue), Os (light blue), Ir (light blue), Pt (light blue), Au (light blue), Hg (light blue), Tl (pink), Pb (pink), Bi (pink), Po (pink), At (pink), Rn (pink), Fr (yellow), Ra (blue), Rf (light blue), Db (light blue), Sg (light blue), Bh (light blue), Hs (light blue), Mt (light blue), Ds (light blue), Rg (light blue), Cn (light blue), Nh (pink), Fl (pink), Mc (pink), Lv (pink), Ts (pink), Og (pink), La (pink), Ce (pink), Pr (pink), Nd (pink), Pm (pink), Sm (pink), Eu (pink), Gd (pink), Tb (pink), Dy (pink), Ho (pink), Er (pink), Tm (pink), Yb (pink), Lu (pink), Ac (pink), Th (pink), Pa (pink), U (pink), Np (pink), Pu (pink), Am (pink), Cm (pink), Bk (pink), Cf (pink), Es (pink), Fm (pink), Md (pink), No (pink), Lr (pink).
- Search Criteria:** Radio buttons for 'Boolean', 'Yes/No/Maybe', and 'Composition List'. Checkboxes for 'And', 'Or', 'Not', 'Only', and 'Just'. A 'Grouping' section with 'And' and 'Or' radio buttons and a '+' icon.
- Bottom Bar:** 'Search', 'Reset Tab', 'Reset All' buttons, 'Range Input' and 'Global Operator' dropdowns, and a search input field.

Search Window

Subfiles/Database Filters

Search

Subfile

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Range Input

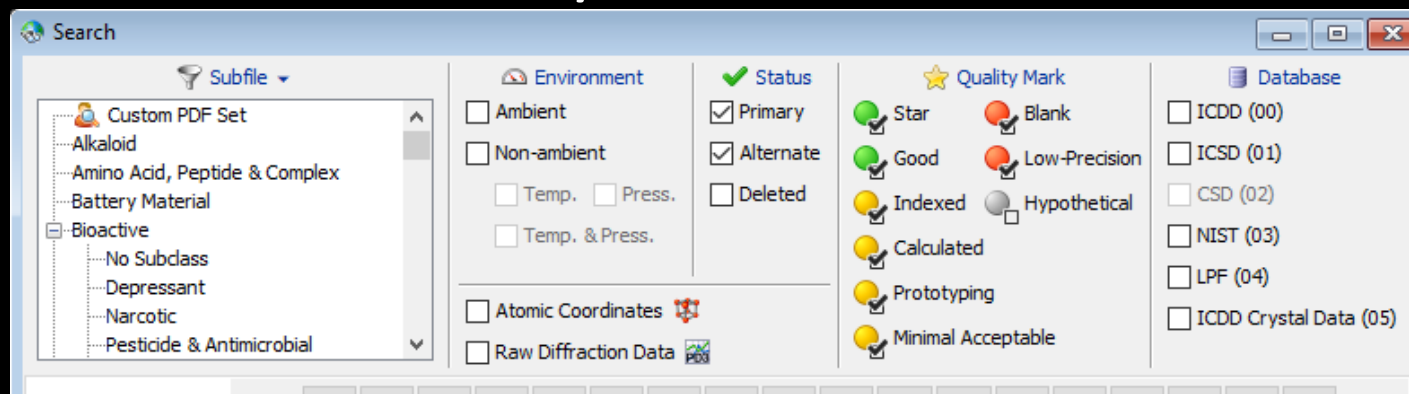
Global Operator

Search Reset Tab Reset All

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

The screenshot shows the ICDD Search Window interface. It includes a 'Subfile' dropdown, a tree view of 'Custom PDF Set' (Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial), and several filter 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 is a 'Periodic Table' section with a grid of elements. A red arrow points to the 'Boolean' radio button in the 'Periodic Table' section, which is selected. Other options include 'Yes/No/Maybe', 'Composition List', 'And', 'Or', 'Not', 'Only', 'Just', and 'Grouping: And, Or'. At the bottom, there are 'Range Input' and 'Global Operator' dropdowns, and buttons for 'Search', 'Reset Tab', and 'Reset All'.

Refine your search by selecting filters based upon the elements in a material. Select elements individually (i.e., *H*, *He*, *Li*, etc.) or by group (i.e., *IA*, *Noble Gases*, *Period 1*, etc.).

Select the *Inner Operator* to combine the elements in the group using *Not*, *And*, *Or*, *Only* and *Just*.

Select the *Outer Operator* to combine element groups using *And* & *Or*.

Search Window

Periodic Table Filters

The screenshot displays the ICDD Search Window with various filters and a periodic table. The filters are organized into several sections:

- Subfile:** A tree view showing categories like Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, and Pesticide & Antimicrobial.
- Environment:** Checkboxes for Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, and Raw Diffraction Data.
- Status:** Checkboxes for Primary, Alternate, Deleted, and a Composition List dropdown.
- Quality Mark:** Checkboxes for Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision.
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), and LPF (04).

The periodic table is shown with elements color-coded based on the search results. A red arrow points to the 'Yes/No/Maybe' radio button in the Composition List dropdown.

Periodic Table	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Formula/Name	1 H																	
Classifications	2 Li	4 Be											5 B	6 C	7 N			
Crystallography	3 Na	12 Mg											13 Al	14 Si	15 P			
Modulated	4 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
Diffraction	5 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
Physical Properties	6 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
Reference	7 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
Comments	La		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
	Ac		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Search Reset Tab Reset All Range Input Global Operator

For the **Yes/No/Maybe** search, click an element to cycle through these three states:

Yes - This element must exist in the pattern (white)

No - This element must not exist in the pattern (black)

Maybe - This element may exist in the pattern (colored)

Search Window

Periodic Table Filters

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

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

Search

Subfile

Custom PDF Set

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

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)

microbial

Boolean ☐ Yes/No/Maybe ☒ Composition List

Select 2-5 elements

Periodic Table: Elements Fe and Ni are highlighted.

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

Comments

Search Reset Tab Reset All

Range Input

Global Operator

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
- Periodic Table**
- Formula/Name:**
 - Formula:** Any Formula
 - Name:** Any Name
- Classifications**
- Crystallography**
- Modulated**
- Diffraction**
- Physical Properties**
- Reference**
- Comments**
- IMA No.:**
- CAS No.:**
- Number of Elements:** Low, High
- Molecular Wt (g/mol):** Value, ±Error
- Composition:** Element, Weight %, ±Error
- Status:** Primary, Alternate, Deleted
- Environment:** Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data
- Range Input:**
- Global Operator:**
- Buttons:** Search, Reset Tab, Reset All

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

Chemical Formula – filters based on the molecular formula.

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

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

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

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

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

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

Search Window

Formula/Name

Search

Subfile

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

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

Search Reset Tab Reset All

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.

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

Search Window

Classifications

The screenshot shows 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 'Ambient', 'Non-ambient', and 'Temp. & Press.'. The 'Status' panel has 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' panel features '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' (AEN - Aenigmatite, ALC - Allactite, VRL - Alluaudite), 'Zeolite Classification' (ABW - Li-A(BW), ACO - ACP-1, AEI - AIPO4-18), and 'Organic Functional Group' (>4_Hetero_atoms_in_ring(s), >5_fused_rings, >9_membered_ring). The bottom of the window has a 'Search' button, 'Reset Tab', 'Reset All', 'Range Input', and 'Global Operator'.

Refine your search by selecting filters based upon classification criteria. The classifications are displayed in a List Criteria Panel. Subclasses are indicated next to a classification by a + button. Single-click this button to expand the list.

Mineral Classification – filters based on the mineral classification.

Zeolite Classification – filters based on the zeolite classification.

Organic Functional Group – filters based on organic functional group.

Search Window

Pearson Symbol Code

Search

Subfile

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Mineral Classification

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

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

Prototype Structure

Any Prototype Structure

Formula Type (ANX)

Wyckoff Sequence

Range Input

Global Operator

Search Reset Tab Reset All

Filters for Pearson Symbol Codes with and without Hydrogen.

Filters based on a user-constructed Pearson Symbol Code.

Search Window

Crystallography

The screenshot displays the 'Search' window in the ICDD software. The 'Crystallography' tab is selected in the left sidebar. The main area contains several filter sections: 'Subfile' with a tree view of categories like 'Alkaloid' and 'Bioactive'; 'Environment' with checkboxes for 'Ambient', 'Non-ambient', and 'Atomic Coordinates'; 'Status' with checkboxes for 'Primary', 'Alternate', and 'Deleted'; 'Quality Mark' with checkboxes for 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', and 'Minimal Acceptable'; 'Database' with checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'; 'Crystal System' with checkboxes for 'Tridinic (Anorthic)', 'Monoclinic', 'Orthorhombic', 'Tetragonal', 'Rhombohedral', 'Hexagonal', and 'Cubic'; 'Crystal (Symmetry Allowed)' with checkboxes for 'Centrosymmetric', 'Non-centrosymmetric', 'Enantiomorphic', 'Pyro / Piezo (p)', and 'Optical Activity'; 'Space Group' with a 'Space Group Symbol' input field; and 'AET' with a dropdown menu. At the bottom, there are four tabs: 'Crystal Data', 'Reduced Cell', 'Author's Unit Cell', and 'Supercell/Subcell'. These four tabs are circled in red. A text box is overlaid on the bottom right of the window, containing the following text:

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

Search Window

Crystal Data

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
- ☐ Hypothetical

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

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

Crystal (Symmetry Allowed)

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

AET

AET

Elements

Space Group

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

Unit Cell

Supercell

Angles (°)

Volume (Å³)

Axial Ratio

c/a: Value ±Error

a/b: Value ±Error

c/b: Value ±Error

Search Reset Tab Reset All Global Operator

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

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

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

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

Search Window

Crystal Data

Search

Subfile

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

- ☐ 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

Axis (Å)

a: Value ±Error

b: Value ±Error

c: Value ±Error

Angles (°)

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume (Å³)

Value ±Error

Axial Ratio

c/a: Value ±Error

c/b: Value ±Error

c/c: Value ±Error

Filters based on the volume of the crystal data.

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

Range Input

Global Operator

Search Reset Tab Reset All

ICDD

INTERNATIONAL CENTRAL FOR DIFFRACTION DATA

ISO 9001:2015

QUALITY MANAGEMENT SYSTEM CERTIFIED

BY DEKRA

CEP-100

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

Hypothetical

Database

ICDD (00)

ICSD (01)

CSD (02)

NIST (03)

LPF (04)

ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Crystal System

Tridinic (Anorthic)

Monoclinic

Orthorhombic

Tetragonal

Rhombohedral

Hexagonal

Cubic

Crystal (Symmetry Allowed)

Centrosymmetric

Non-centrosymmetric:

Enantiomorphic

Pyro / Piezo (p)

Optical Activity

Piezo (2nd Harm.)

AET

AET

Elements

Space Group

Space Group Symbol

Crystal Data

Reduced Cell

Author's Unit Cell

Supercell/Subcell

Axis (Å)

a: Value ±Error

b: Value ±Error

c: Value ±Error

Angles (°)

α: Value ±Error

β: Value ±Error

γ: Value ±Error

Volume (Å³)

Value ±Error

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

The screenshot shows the ICDD Search Window with the 'Author's Cell' section selected. A 'Convert Cell' dialog box is open, showing options to convert from 'Author's Unit Cell' to 'Crystal Data' or 'Reduced Cell'. The dialog is set to 'Tridlinic (Anorthic)' and 'Primitive' Bravais Lattice. The 'Convert to Crystal Data' option is selected.

Convert Cell

Crystal System: Tridlinic (Anorthic)
 Bravais Lattice: Primitive
 ☒ Convert to Crystal Data
 ☐ Convert to Reduced Cell
 [Convert] [Cancel]

Search Window - Author's Cell Section

Axis (Å)

Axis	Value	±Error
a:	Value	±Error
b:	Value	±Error
c:	Value	±Error

Angles (°)

Angle	Value	±Error
α:	Value	±Error
β:	Value	±Error
γ:	Value	±Error

Volume (Å³)

Volume	Value	±Error
Value	Value	±Error

Molecular/f.u. Volume

Volume	Value	±Error
Value	Value	±Error

Axial Ratio

Ratio	Value	±Error
c/a:	Value	±Error
a/b:	Value	±Error
c/b:	Value	±Error

Annotations:

- 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. A red arrow points from the text box to the 'Supercell/Subcell' tab in the 'Crystal Data' section.

Search Window Interface:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide, & 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
 - ☐ Hypothetical
- 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**
- Supercell/Subcell Options:**
 - Axis (Å):
 - a: Value ±Error
 - b: Value ±Error
 - c: Value ±Error
 - Angles (°):
 - α: Value ±Error
 - β: Value ±Error
 - γ: Value ±Error
 - ☒ Supercell
 - ☐ Subcell
 - Volume Ratio: 1 to 1
- Bottom Bar:**
 - Search Reset Tab Reset All
 - 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
- ☒ Blank
- ☒ Prototyping
- ☒ Minimal Acceptable

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 Subsystems)

Range Input

Global Operator

Search Reset Tab Reset All

Filters based on the number of dimensions used to describe the modulation where "3 + 1d", "3 + 2d", "3 + 3d" indicate one, two, and three additional dimensions respectively.

Filters patterns based on the number of subsystems present in the structure. Composite structures have more than one subsystem.

Search Window

Diffraction

Search

Subfile

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

Environment

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

Status

- ☒ Primary
- ☒ Alternate
- ☐ Deleted

Quality Mark

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

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Radiation: ☒ X-ray/Electron ☐ CW Neutron

Strong Line (Å)

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

Range Input

Global Operator

Search Reset Tab Reset All

Filters based on the ratio of the intensity of the strongest line of the pattern to the intensity of the strongest line of corundum in a 50/50 weight mixture.

Filters based on the SS/FOM. The figure of merit generally used is that reported by Smith & Snyder, which indicates the completeness & accuracy of measured interplanar spacings.

Search Window

Physical Properties

Search

Subfile

Custom PDF Set

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

Environment

Ambient

Non-ambient

Temp. Press.

Temp. & Press.

Atomic Coordinates

Raw Diffraction Data

Status

Primary

Alternate

Deleted

Quality Mark

Star

Good

Indexed

Calculated

Prototyping

Minimal Acceptable

Blank

Low-Precision

Hypothetical

Database

ICDD (00)

ICSD (01)

CSD (02)

NIST (03)

LPF (04)

ICDD Crystal Data (05)

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Melting Point (K)

Value

±Error

Density (g/cm³)

Value

±Error

Measured Density

Calculated

Not

Property Sheet

Topology

Topology vdW Volume (Å³)

Value

±(%)

Topology Total Porosity (Å)

Value

±(%)

Color

Black

Blue

Brown

Color Missing

Colorless

Filters based on the measured, calculated or structural density of the material.

Filters based on the melting point. Specify degrees Celsius, Kelvin or Fahrenheit by selecting from the drop down menu.

Range Input

Global Operator

Search Reset Tab Reset All

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

Volume

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
- ☐ Hypothetical

Database

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

Periodic Table

Formula/Name

Classifications

Crystallography

Modulated

Diffraction

Physical Properties

Reference

Comments

Database Comments

Filter based on the text contained in comments.

Absolute Configuration:
Additional Diffraction Lines:
Additional Patterns:
Analysis:
ANX:
Atomic Position:
Bioactivity:
Boiling Point:

Search Reset Tab Reset All

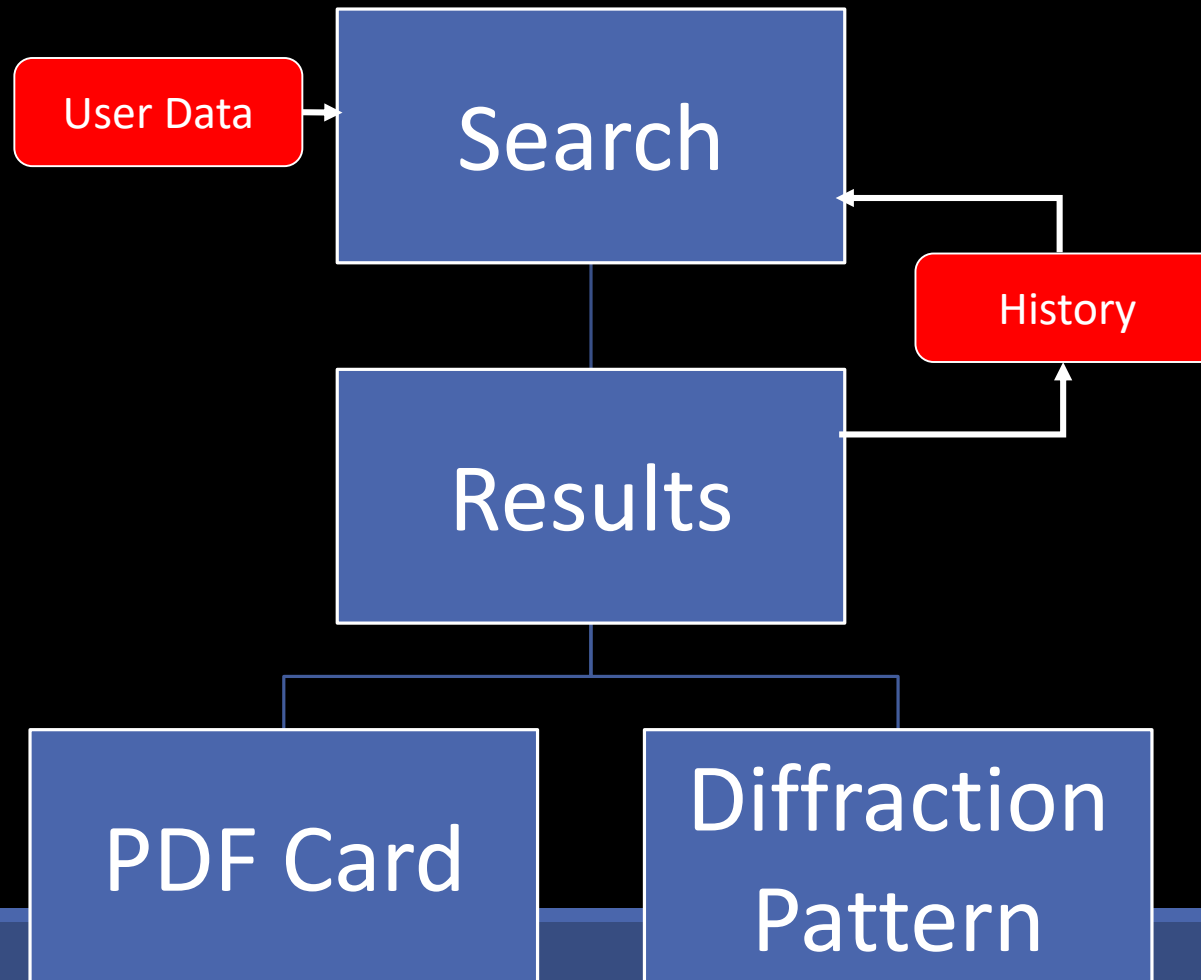
Range Input

Global Operator

Data Mining Basics

- Select your filter criteria
- Make use of logical Boolean operators, text and list boxes
- Search
- Review results
- Refine search with additional criteria

Note: Selected search criteria is highlighted in red to keep track of your selections.



Select
Elements in
Periodic Table

Search Example

The image displays three screenshots of the ICDD search interface, illustrating the steps to perform a search. Red boxes and arrows highlight the specific actions being performed.

Top Screenshot: The 'Periodic Table' tab is selected. The elements H, Be, Na, and Mg are highlighted in the periodic table. A red arrow points from the 'Select Elements in Periodic Table' text to the highlighted elements.

Bottom Left Screenshot: The 'Crystallography' tab is selected. The 'Space Group' dropdown menu is open, and 'P4/mmm' is selected. A red arrow points from the 'Select Space Group' text to the selected space group.

Bottom Right Screenshot: The 'Formula/Name' field is populated with 'Potassium Platinum Chloride'. A red arrow points from the 'Select Compound Name' text to the entered name.

Selected filters highlighted in red: The 'Status' filters 'Primary', 'Alternate', and 'Deleted' are highlighted in red. The 'Quality Mark' filters 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', and 'Minimal Acceptable' are also highlighted in red.

Search Query: The search query is displayed at the bottom: `[[Pt And Cl]] And [Any Name Contains Fragments 'Potassium' And 'Platinum' And 'Chloride']] And [Space Group Symbol Contains Phrase 'P4/mmm']] And [Exclude Deleted/Hypothetical Patterns]]`

Search Results

Choose fields to be displayed in results

Results - 9 of 460,954

File Fields Tools

Open PDF Card Simulated Profile

My Defaults

Search Results

PDF #	QM	Chemical Formula	Compound Name	Coords	Weight %	D1 (Å)	D2 (Å)	D3 (Å)	SYS	SG #
00-009-0367	I	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	6.940	3.160	3.550	T	123
01-073-1506	I	$K_2(PtCl_4)$	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	6.990000	3.169250	3.555730	T	123
04-006-6128	P	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	7.024000	3.183270	3.571050	T	123
04-007-2797	S	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	7.023000	3.183810	3.571940	T	123
04-007-5356	I	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	7.025000	3.182100	3.569270	T	123
04-007-7303	S	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	6.996100	3.159080	3.540590	T	123
04-007-7304	S	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	6.981300	3.156210	3.538480	T	123
04-009-8290	B	K_2PtCl_4	Potassium Platinum Chloride	✓	Cl34.16 K18.84 Pt47.00	7.024000	3.183270	3.571050	T	123
04-013-8855	B	$K_2Pt(CN)_4Cl_{0.32}(H_2O)_{2.6}$	Potassium Platinum Chloride Cyanide Hydrate	✓	C11.03 Cl2.60 H1.20 K17.95 N12.86 O9.55 Pt44.79	9.866000	4.412210	6.976320	T	123

[(Pt And Cl)] And [Any Name Contains Fragments 'Potassium' And 'Platinum' And 'Chloride'] And [Space Group Symbol Contains Phrase 'P4/mmm'] And [Exclude Deleted/Hypothetical Patterns]

Search Filters

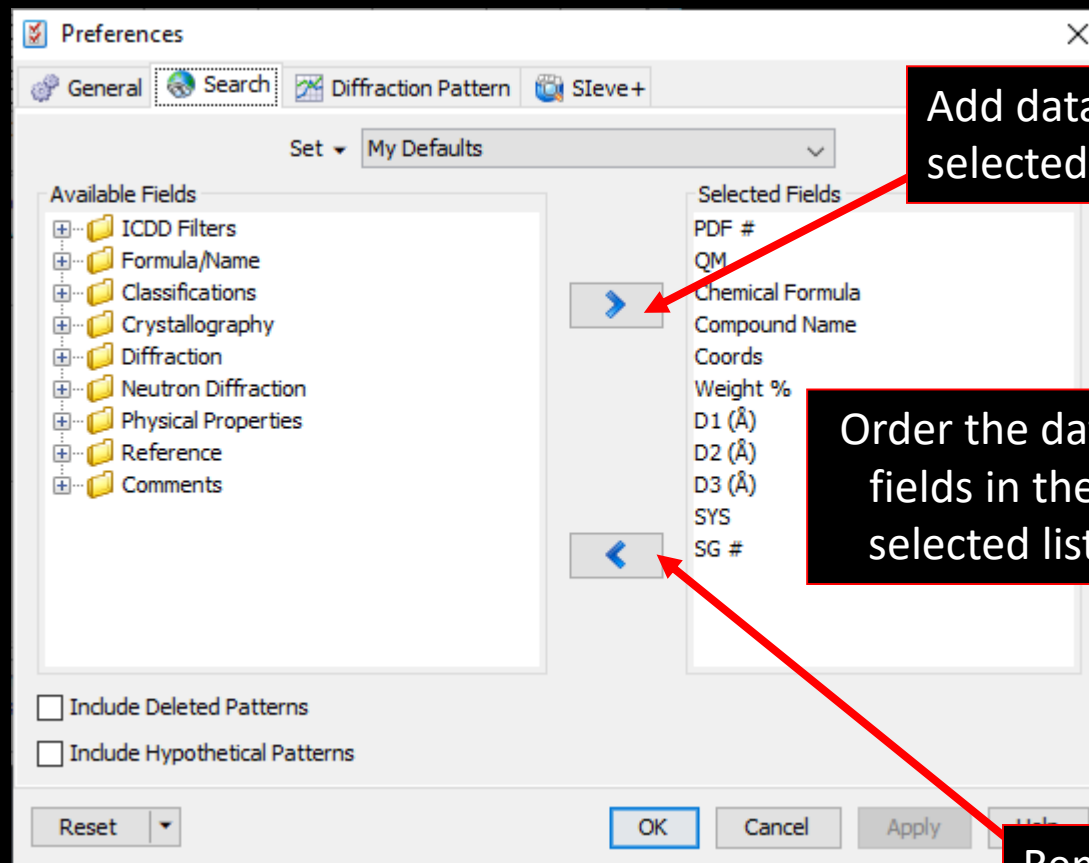
Double-click on a PDF number to view the entire PDF Card



Preferences Module

Open the Preferences Module to select which data fields you would like to display in your results.

You can also select the order in which the data fields are displayed.



Add data fields to selected list

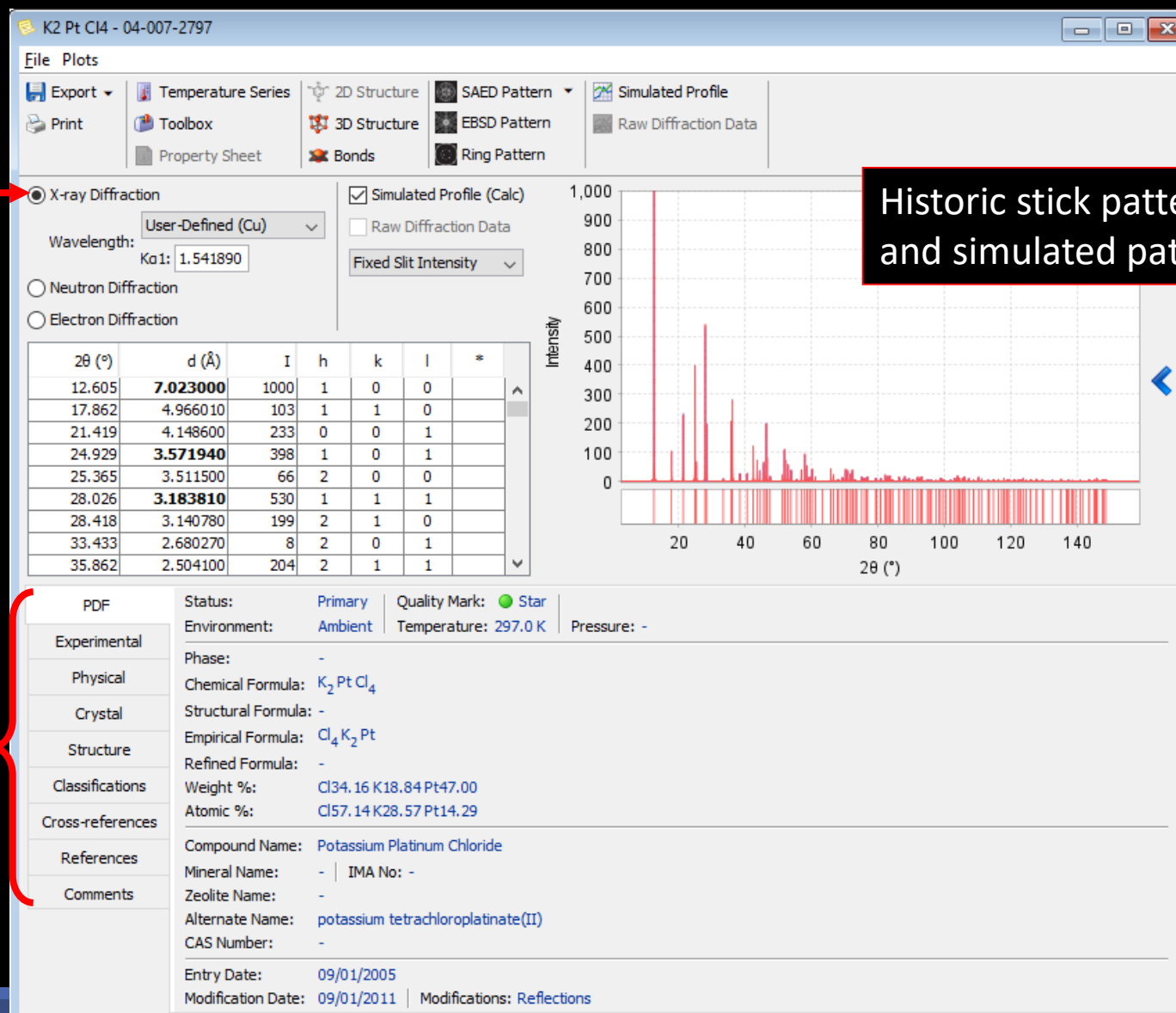
Order the data fields in the selected list

Remove data fields from the selected list

PDF Data Card

Choose
equipment
factors

Historic stick pattern
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 460,954

Fields Tools

Open PDF Card Simulated Profile

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

Open PDF Card

Tools/Simulations

Add to Custom PDF Set...

Remove from Custom PDF Set...

Copy Chemical Formula

Remove Rows

[(Pt And Cl)] And [Any Name Contains Fragments 'Potassium' And 'Platinum' And 'Chloride']

K2 Pt Cl4 - 04-007-7303

File Plots

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

Tools

Property Sheet

3D Structure EBSD Pattern Ring Pattern

Wavelength: User-Defined

Ko1: 1.54056 Å

2θ (°)

12.653 6.99

17.931 4.9

21.649 4.1

25.153 3.54

25.464 3.4

28.250 3.15

28.530 3.1

33.663 2.6

36.096 2.4

PDF

Experimental

Physical

Crystal

Structure

Classifications

Cross-references

References

Comments

K2 Pt Cl4 - 01-073-1506

File Plots

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

Tools

Property Sheet

3D Structure EBSD Pattern Ring Pattern

Wavelength: User-Defined

Ko1: 1.54056 Å

2θ (°)

12.664 6.990

17.947 4.94

21.517 4.13

25.044 3.555

25.487 3.49

28.158 3.169

28.555 3.12

33.593 2.66

36.034 2.49

PDF

Experimental

Physical

Crystal

Structure

Classifications

Cross-references

References

Comments

K2 Pt Cl4 - 00-009-0367

File Plots Help

Export Print

Temperature Series 2D Structure SAED Pattern Simulated Profile

Tools

Property Sheet

3D Structure EBSD Pattern Ring Pattern

Wavelength: Cu Ko1 1.54056 Å

2θ (°)

12.745 6.940

17.978 4.930

21.551 4.120

25.063 3.550

25.502 3.490

28.217 3.160

28.586 3.120

33.536 2.670

36.055 2.489

36.281 2.474

PDF

Experimental

Physical

Crystal

Structure

Classifications

Cross-references

References

Comments

Status: Primary

Environment: Ambient

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: -

Simulated Profile (Exp-based)

Raw Diffraction Data

Fixed Slit Intensity

Intensity

2θ (°)

5 10 15 20 25 30 35 40 45 50 55 60 65 70

PDF Data Card Features



View Temperature Series

Results - 9 of 460,954

File Fields Tools

Open PDF Card Simulated Profile

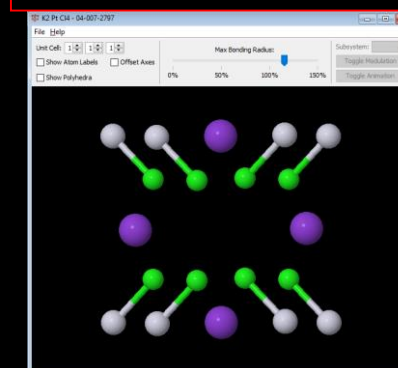
Temp (K)	Pressure (GPa)	PDF #	QM	Chemical Formula	Compound Name	RedCell Vol (Å ³)	Author - PR	Journal - PR	Year - PR	Dcalc (g/cm ³)	Dstruc (g/cm ³)
120.0		04-007-7303	S	K ₂ PtCl ₄	Potassium Platinum Chloride	200.93	Takazawa H., Ohba S., Saito Y., Sano M.	Acta Crystallogr., Sect. B: Struct. Sci.	1997	3.43	3.43
120.0		04-007-7304	S	K ₂ PtCl ₄	Potassium Platinum Chloride	200.06	Takazawa H., Ohba S., Saito Y., Sano M.	Acta Crystallogr., Sect. B: Struct. Sci.	1997	3.445	3.44
293.0	1.01E-4	04-007-5356	I	K ₂ PtCl ₄	Potassium Platinum Chloride	204.51	Maier R.H.B., Ovston P.G., Wood A.M.	Acta Crystallogr., Sect. B: Struct. Crystallogr., Cryst. Chem.	1972	3.37	3.37
297.0		04-007-2797	S	K ₂ PtCl ₄	Potassium Platinum Chloride	204.62	Ohba S., Sato S., Saito Y., Ohshima K., Harada J.	Acta Crystallogr., Sect. A: Found. Crystallogr.	1985	3.369	3.37
297.0		04-009-8290	B	K ₂ PtCl ₄	Potassium Platinum Chloride	204.60	Ohba S., Sato S., Saito Y., Ohshima K., Harada J.	Acta Crystallogr., Sect. B: Struct. Sci.	1983	3.369	3.37
298.0		00-001-0102	I	K ₂ PtCl ₄	Potassium Platinum Chloride	201.79	Hanawalt, J., et al.	Anal. Chem.	1938	3.416	
298.0		00-009-0367	I	K ₂ PtCl ₄	Potassium Platinum Chloride	201.96	Staritzky.	Anal. Chem.	1956	3.413	
298.0		01-073-1506	I	K ₂ (PtCl ₄)	Potassium Platinum Chloride	201.79	Dickinson, R.G.	J. Am. Chem. Soc.	1922	3.416	3.415
298.0		04-006-6128	P	K ₂ PtCl ₄	Potassium Platinum Chloride	204.60	Ohba S., Matsuda T., Hattai I., Harada J.	J. Phys. Soc. Jpn.	1981	3.369	3.37

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

View Bond Distances/Angles



View 3D Structure



View Toolbox

Toolbox

Settings

Wavelength: User-Defined (Cu) Ka1: 1.541890

a (Å): 7.023 a (°): 90

b (Å): 7.023 b (°): 90

c (Å): 4.1486 c (°): 90

Calculate Peak

h: ☐ i: ☐ 2θ: ☐

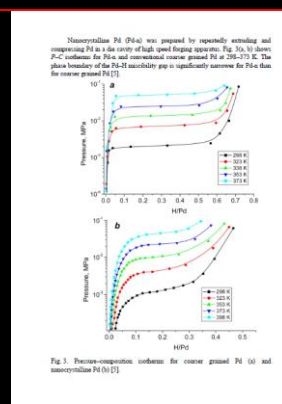
h₂: ☐ k₂: ☐ d-spacing: ☐

Calculate Peak List

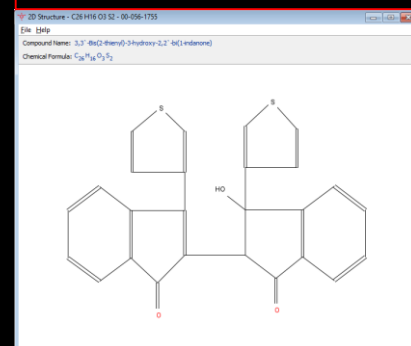
Start 2θ (°):

Stop 2θ (°):

View Property Sheet



View 2D Structure

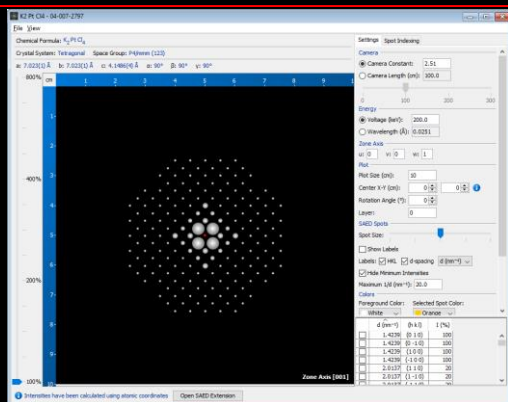


Note: The availability of each feature varies by PDF entry.

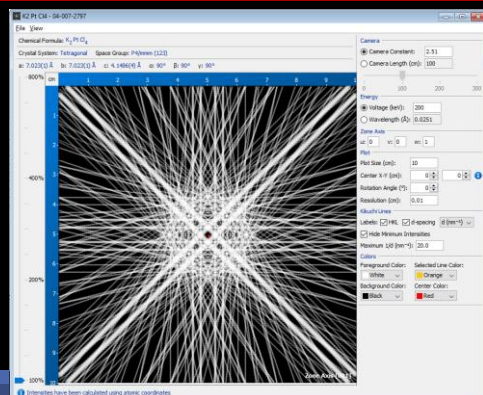
PDF Data Card Features



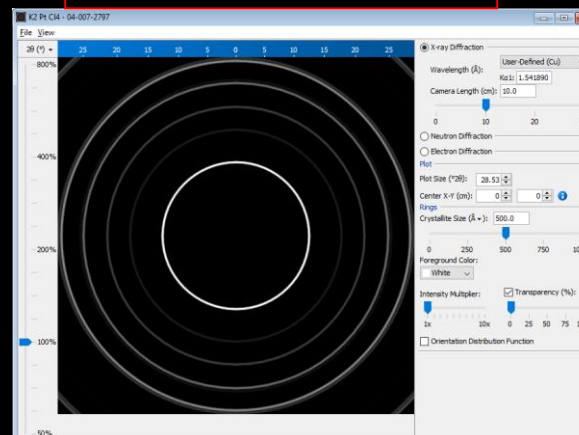
View Simulated Electron Spot Pattern



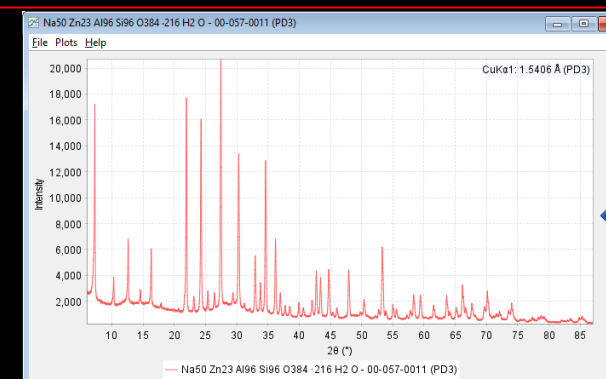
View Electron Backscattering Pattern



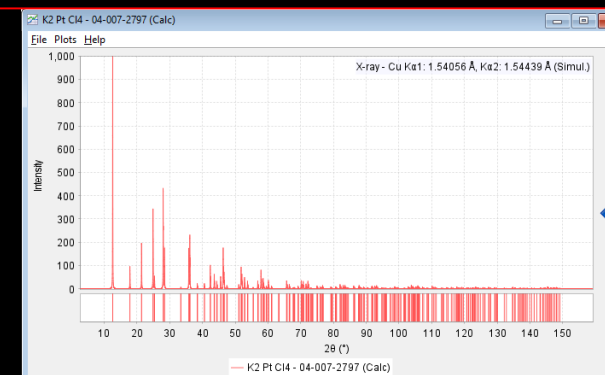
View Ring Pattern



View Raw Diffraction Data (PD3)



View Simulated Diffraction Profile





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