

PDF-4+ Tools and Searches



PDF-4+ 2018

The PDF-4+ 2018 database is powered by our integrated search display software. PDF-4+ 2018 boasts 72 search selections coupled with 125 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+ 2018.

PDF-4+ 2018

File Edit Window Help

Open PDF Cards Preferences Search History Results Sieve+ Microanalysis

Search

Subfile

Custom PDF Set

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

Environment

- Ambient
- Press. (Non-ambient)
- Temp. (Non-ambient)
- Press. & Temp. (Non-ambient)
- 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

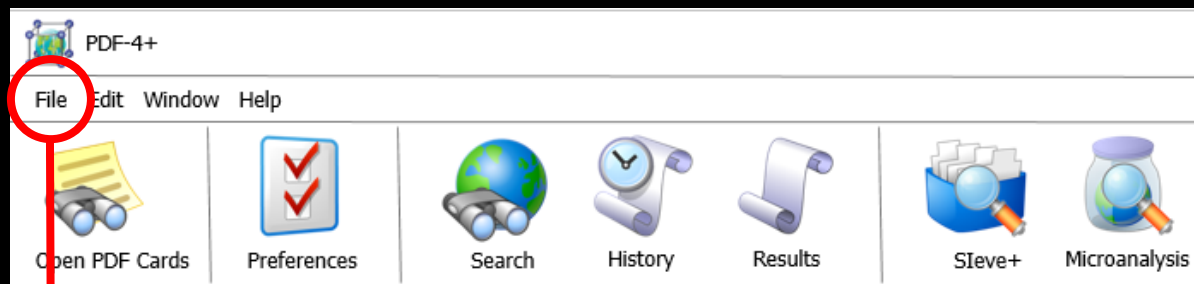
	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA		
Formula/Name	1 H 1.008															2 He 4.003		
Classifications	3 Li 6.941	4 Be 9.012									5 B 10.811	6 C 12.01	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180		
Crystallography	11 Na 22.990	12 Mg 24.305									13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.065	17 Cl 35.453	18 Ar 39.948		
Modulated																		
Diffraction	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 58.993	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
Physical Properties	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
Reference	55 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]
Comments	87 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]
			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	
			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]	

Search Reset Tab Reset All Help Numeric Input Global Operator

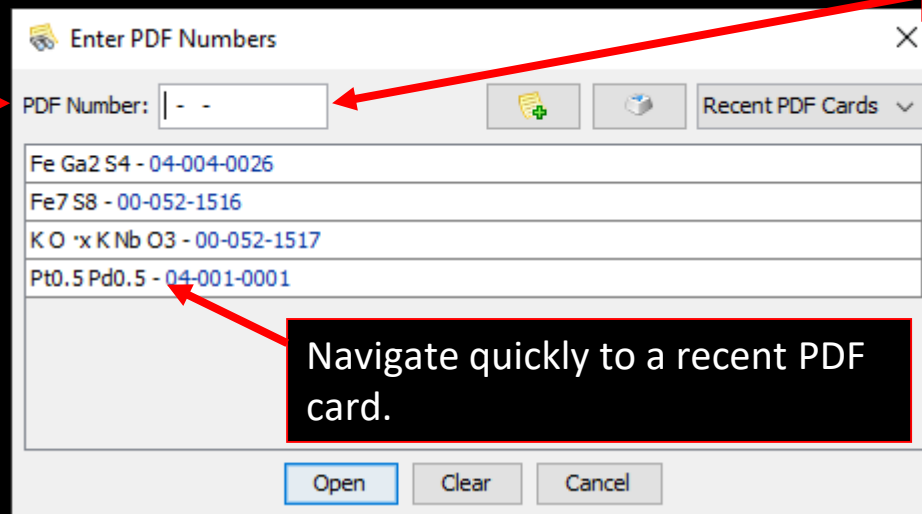
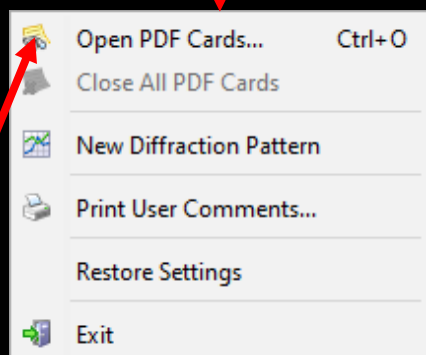
Tool Bar

Primary Search Menu

Getting Started

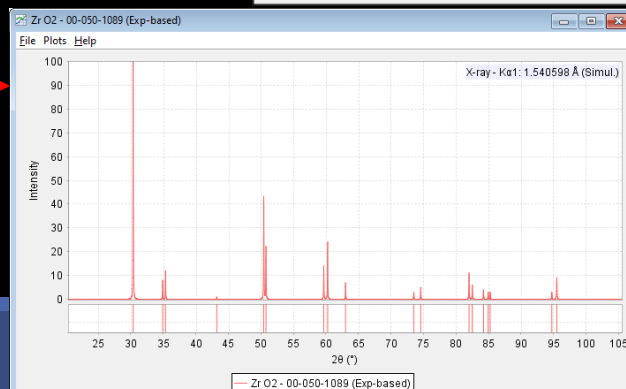


Open a known PDF card.

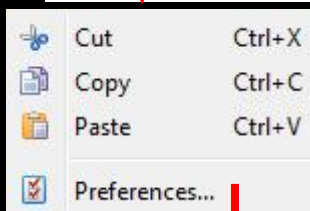
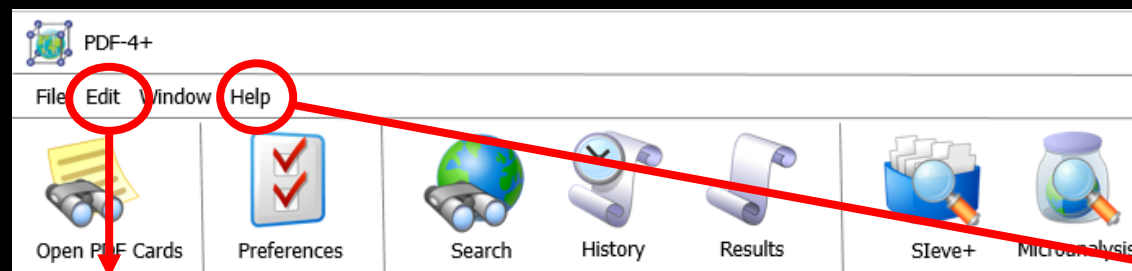


Navigate quickly to a recent PDF card.

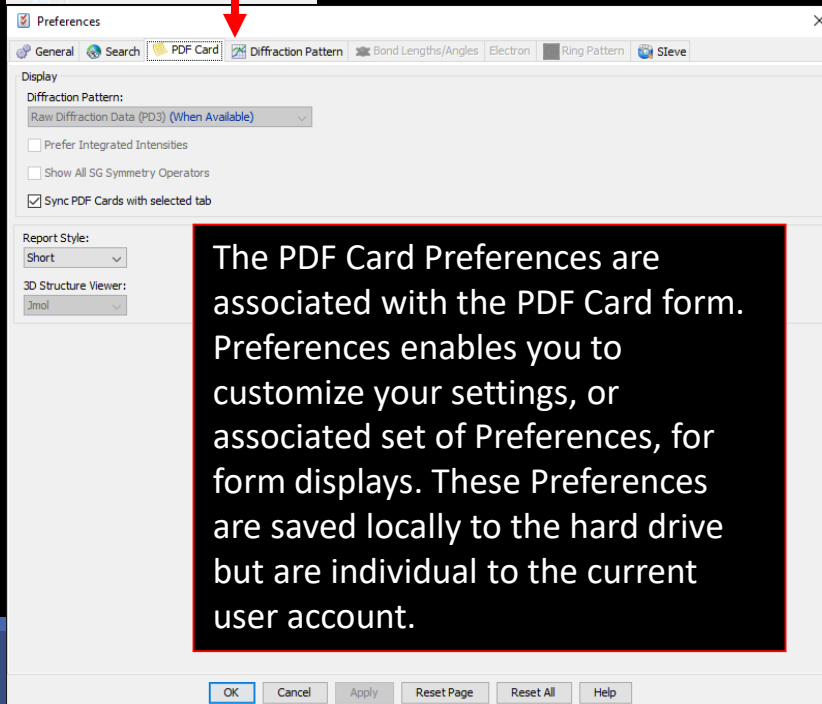
Open a previously saved diffraction pattern. The pattern must be of the ICDD XML file format. All PDF entries can be saved in this format.



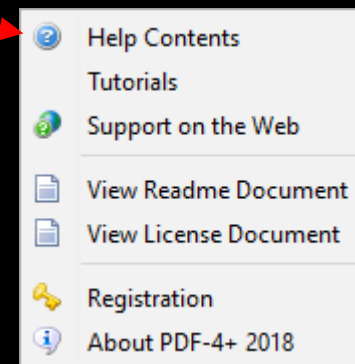
Getting Started



Edit functions



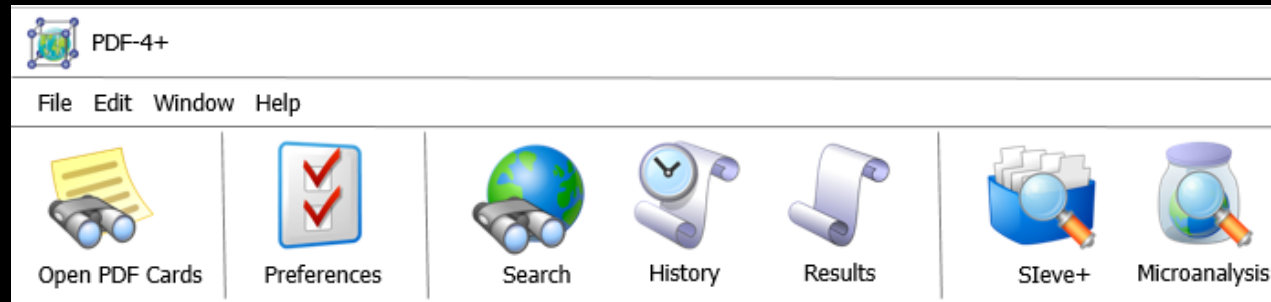
The PDF Card Preferences are associated with the PDF Card form. Preferences enables you to customize your settings, or associated set of Preferences, for form displays. These Preferences are saved locally to the hard drive but are individual to the current user account.



Help information regarding use, support, license policy, and registration of the PDF-4+. Be sure to register the PDF-4+ by clicking on Registration within 10 days of installation to activate the full license term.

Customize Wavelength, Intensity, Report Style, and many more features of the PDF-4+.

Tool Bar



Quick Navigation Icons



Select a PDF Card



Select Preferences Module



Open Search Window



Microanalysis



Open History Window



Open Results Window



Open Sieve+

Primary Search Menu

The Search Window displays nine tabs. Each tab features multiple search criteria to allow you to data mine the PDF-4+. Searching the PDF-4+ is an iterative process that allows you to input user-defined criteria, view the results, and combine additional criteria to refine your results.

The screenshot shows the ICDD Primary Search Menu interface. The window is titled "Search" and contains several panels for filtering search results:

- Subfile:** A tree view showing categories like "Alkaloid", "Amino Acid, Peptide & Complex", "Battery Material", "Bioactive", "No Subclass", "Depressant", "Narcotic", and "Pesticide & Antimicrobial".
- Environment:** Checkboxes for "Ambient", "Press. (Non-ambient)", "Temp. (Non-ambient)", "Press. & Temp. (Non-ambient)", "Atomic Coordinates", and "Raw Diffraction Data".
- Status:** Checkboxes for "Primary", "Alternate", and "Deleted".
- Quality Mark:** A legend with color-coded markers for "Star", "Good", "Indexed", "Calculated", "Prototyping", "Minimal Acceptable", "Blank", and "Low-Precision".
- Database:** Checkboxes for "ICDD (00)", "ICSD (01)", "CSD (02)", "NIST (03)", "LPF (04)", and "ICDD Crystal Data (05)".

Below the panels is a periodic table with search criteria applied to various elements. The search criteria are:

- Formula/Name: Boolean Search (selected), Yes/No/Maybe Search
- Classifications: Set Unselected to No

The periodic table shows elements with their atomic numbers, symbols, and names. Elements are highlighted in various colors (green, yellow, blue, red, purple, cyan) based on the search criteria. For example, H, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in red. Elements like B, C, N, O, F, Ne, Al, Si, P, S, Cl, Ar, Ga, Ge, As, Se, Br, Kr, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in yellow. Elements like Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in blue. Elements like H, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in cyan. Elements like H, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in purple. Elements like H, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr are highlighted in red.

At the bottom of the window, there are buttons for "Search", "Reset Tab", "Reset All", and "Help". There are also dropdown menus for "Numeric Input" and "Global Operator".

Search Window

Subfiles/Database Filters

The screenshot shows the 'Search' window with several filter panels:

- 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, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, and Raw Diffraction Data (PD3).
- Status:** Checkboxes for Primary, Alternate, and Deleted.
- Quality Mark:** A list of quality levels: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision.
- Database:** Checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05).

Below the filters is a periodic table with columns labeled IA through VIIIA. A search box is overlaid on the table with the following text:

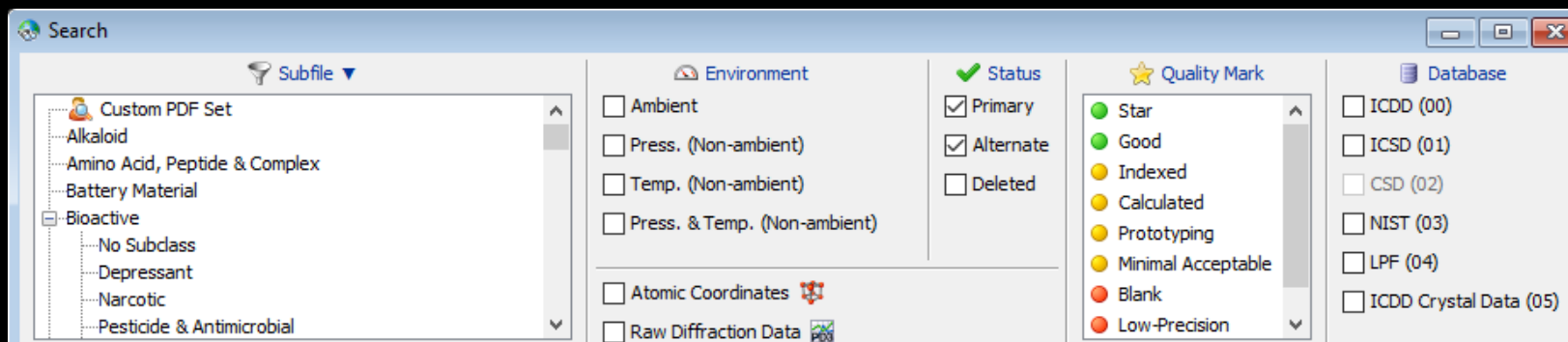
Boolean Search Yes/No/Maybe Search
Set Unselected to *No*

At the bottom of the window are buttons for Search, Reset Tab, Reset All, and Help, along with a numeric input field and a global operator dropdown.

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 displays the ICDD Search Window interface. On the left, there is a 'Subfile' dropdown menu with a tree view containing categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. To the right of this are filter sections for 'Environment' (Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data), 'Status' (Primary, Alternate, Deleted), and 'Quality Mark' (Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision). Below these filters is a search control area with radio buttons for 'Boolean Search' (selected) and 'Yes/No/Maybe Search', and options for 'And', 'Or', 'Not', 'Only', and 'Just' operators. A red arrow points from the 'Just' operator to the 'Quality Mark' section. The main part of the window is a periodic table with elements color-coded by group. The bottom of the window features a search bar, 'Reset Tab', 'Reset All', and 'Help' buttons, along with 'Numeric Input' and 'Global Operator' dropdowns.

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 Search Window interface includes the following sections:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial).
- Environment:** Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), 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).

The Periodic Table is displayed with columns IA through IVA. Search options include Boolean Search and Yes/No/Maybe Search. A text box allows setting unselected elements to 'No'.

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

Formula/Name

The screenshot shows the 'Search' window with the 'Formula/Name' section selected. The 'Formula' dropdown menu is open, showing the following options:

- Any Formula
- Chemical Formula
- Empirical Formula
- Structural Formula
- Contains Elements
- Contains Phrase
- Exactly
- Not

The 'Formula' dropdown is currently set to 'Any Formula'. The search criteria are: 'Any Formula' for the Formula field and 'Any Name' for the Name field. The 'Number of Elements' is set to 'Low' to 'High'. The 'Composition' section is expanded, showing 'Element', 'Weight %', and 'ESD' options.

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

Chemical Formula – filters based on the molecular formula.

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

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

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

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

Search Window

Formula/Name

The screenshot shows the ICDD Search Window with the following sections:

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (expanded), No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial.
- Environment:** Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary (checked), Alternate (checked), 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).
- Search Criteria:** Formula (Any Formula), Name (Any Name), IMA No., CAS Number, Number of Elements (Low/High), Composition (Element/Weight %).
- Left Panel:** Periodic Table, Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, Comments.
- Buttons:** Search, Reset Tab, Reset All, Help, Numeric Input, Global Operator.

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

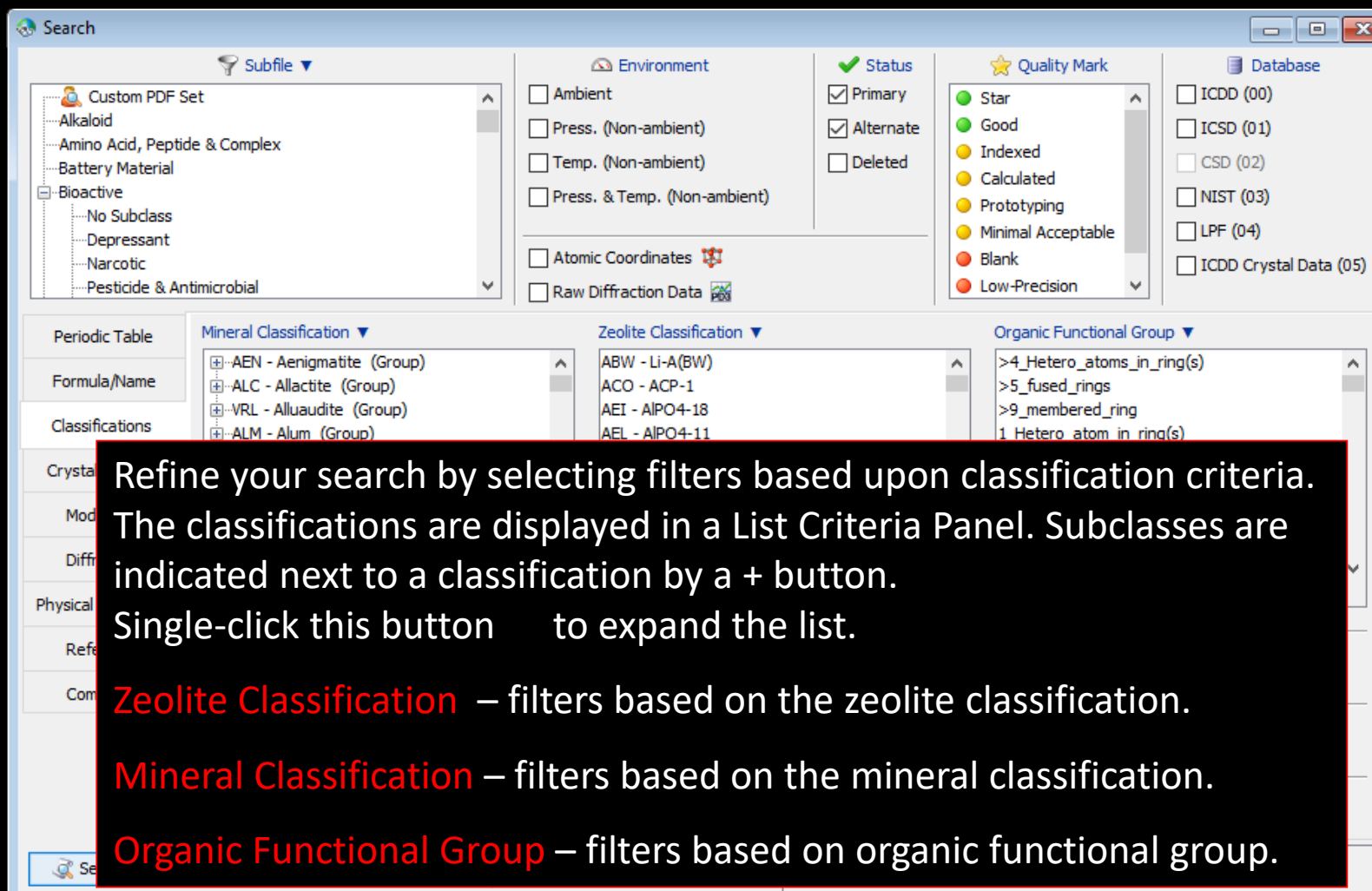
Compound Name – filters based on the compound name.

Mineral Name – filters based on the mineral name.

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

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

Search Window Classifications



The screenshot shows a 'Search' window with several filter panels. The 'Subfile' panel lists categories like 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'. The 'Environment' panel has checkboxes for 'Ambient', 'Press. (Non-ambient)', 'Temp. (Non-ambient)', 'Press. & Temp. (Non-ambient)', 'Atomic Coordinates', and 'Raw Diffraction Data'. The 'Status' panel has checkboxes for 'Primary', 'Alternate', and 'Deleted'. The 'Quality Mark' panel has a list of quality levels: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision. The 'Database' panel has checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'. Below these are three classification panels: 'Mineral Classification' (listing AEN, ALC, VRL, ALM), 'Zeolite Classification' (listing ABW, ACO, AEI, AEL), and 'Organic Functional Group' (listing ring and fused ring counts). A text box is overlaid on the bottom of the window, providing instructions on how to use these 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.

Zeolite Classification – filters based on the zeolite classification.

Mineral Classification – filters based on the mineral classification.

Organic Functional Group – filters based on organic functional group.

Search Window

Pearson Symbol Code

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

- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive (No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial).
- Environment:** Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary (checked), Alternate (checked), 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).
- Mineral Classification:** AEN - Aenigmatite (Group), ALC - Allactite (Group), VRL - Alluaudite (Group), ALM - Alum (Group), ALN - Alunite (Supergroup), AMB - Amblygonite (Group), AMP - Amphibole (Family), ANC - Analcime (Supergroup), ANY - Ancyrite (Supergroup), ADA - Andalusite (Group), ANT - Antlerite (Group).
- Zeolite Classification:** ABW - Li-A(BW), ACO - ACP-1, AEI - AIPO4-18, AEL - AIPO4-11, AEN - AIPO-EN3, AET - AIPO4-8, AFG - Afghanite, AFI - AIPO4-5, AFN - AIPO-14, AFO - AIPO4-41, AFR - SAPO-40.
- Organic Functional Group:** >4_Hetero_atoms_in_ring(s), >5_fused_rings, >9_membered_ring, 1_Hetero_atom_in_ring(s), 1,2_dione____O=C-C=O, 2_fused_rings, 2_Hetero_atoms_in_ring(s), 3_fused_rings, 3_Hetero_atoms_in_ring(s), 3_membered_rinn.
- Pearson Symbol:** With Hydrogen.
- Prototype Structure:** Any Prototype Structure.
- Formula Type (ANX):**

At the bottom, there are buttons for Search, Reset Tab, Reset All, and Help, along with a Numeric Input field and a Global Operator dropdown.

Filters for Pearson Symbol Codes with and without Hydrogen.

Filters based on a user-constructed Pearson Symbol Code.

Search Window Crystallography

Search

Subfile

Custom PDF Set

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

Environment

- Ambient
- Press. (Non-ambient)
- Temp. (Non-ambient)
- Press. & Temp. (Non-ambient)
- 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

- Tridinic (Anorthic)
- Rhombohedral
- Monodinic
- Hexagonal
- Orthorhombic
- Cubic
- Tetragonal

Crystal (Symmetry Allowed)

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

Atomic Environment Type

Symbol	Elements
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

Space Group

Space Group Symbol

Crystal Data

Axis (Å)

Axis	Value	ESD	Angle	Value	ESD	Ratio	Value	ESD	Volume	Value	ESD
a	Value	ESD	α	Value	ESD	c/a	Value	ESD	Volume	Value	ESD
b	Value	ESD	β	Value	ESD	a/b	Value	ESD			
c	Value	ESD	γ	Value	ESD	c/b	Value	ESD			

Search

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

Search Window Crystal Data

Search Window

Subfile

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

Environment

- Ambient
- Press. (Non-ambient)
- Temp. (Non-ambient)
- Press. & Temp. (Non-ambient)
- 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

- Tridinic (Anorthic)
- Monodinic
- Orthorhombic
- Tetragonal
- Rhombohedral
- Hexagonal
- Cubic

Crystal (Symmetry Allowed)

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

Atomic Environment Type

Symbol	Elements
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

Space Group

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

Volume

Value

ESD

Search

Reset Tab

Reset All

Help

Numeric Input

Global Operator

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

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

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

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

Search Window

Crystal Data

Search

Subfile

Custom PDF Set

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

Environment

- Ambient
- Press. (Non-ambient)
- Temp. (Non-ambient)
- Press. & Temp. (Non-ambient)
- 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

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

Crystal (Symmetry Allowed)

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

Atomic Environment Type

Symbol	Elements
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

Space Group

Space Group Symbol

Crystal Data

Axis (Å)	ESD	Angle	ESD	Axial Ratio	ESD	Volume	ESD	
a:	Value	ESD	α :	Value	ESD	c/a:	Value	ESD
b:	Value	ESD	β :	Value	ESD	a/b:	Value	ESD
c:	Value	ESD	γ :	Value	ESD	c/b:	Value	ESD

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

Filters based on the volume of the crystal data.

Search

Reset Tab

Reset All

Help

Numeric Input

Global Operator

Search Window

Reduced Cell

The screenshot shows the ICDD Search Window interface. The window is titled "Search" and contains several sections for filtering search results:

- 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", "Press. (Non-ambient)", "Temp. (Non-ambient)", "Press. & Temp. (Non-ambient)", "Atomic Coordinates", and "Raw Diffraction Data".
- Status:** Checkboxes for "Primary", "Alternate", and "Deleted".
- Quality Mark:** A list of quality marks: Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision.
- Database:** Checkboxes for "ICDD (00)", "ICSD (01)", "CSD (02)", "NIST (03)", "LPF (04)", and "ICDD Crystal Data (05)".
- Crystal System:** Checkboxes for "Tridinic (Anorthic)", "Rhombohedral", "Monoclinic", "Hexagonal", "Orthorhombic", "Cubic", and "Tetragonal".
- Crystal (Symmetry Allowed):** Checkboxes for "Centrosymmetric", "Non-centrosymmetric", "Enantiomorphic", "Pyro / Piezo (p)", "Optical Activity", and "Piezo (2nd Harm.)".
- Atomic Environment Type:** A table with columns "Symbol" and "Elements".
- Space Group:** A dropdown menu for "Space Group" and a text input for "Space Group Symbol".
- Crystal Data:** Input fields for "Reduced Cell", "Author's Cell", and "Supercell/Subcell".
- Axis (Å):** Input fields for "a:", "b:", and "c:" with "ESD" (Error Standard Deviation) fields.
- Volume:** Input fields for "Volume" and "ESD".

At the bottom, there are buttons for "Search", "Reset Tab", "Reset All", and "Help", along with a "Numeric Input" and "Global Operator" dropdown.

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 'Search' window with several filter panels. The 'Environment' panel includes options for Ambient, Press. (Non-ambient), Temp. (Non-ambient), and Press. & Temp. (Non-ambient). The 'Status' panel has checkboxes for Primary, Alternate, and Deleted. The 'Quality Mark' panel lists Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision. The 'Database' panel includes ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05). The 'Crystallography' panel has checkboxes for Monoclinic, Hexagonal, Non-centrosymmetric, Orthorhombic, Cubic, Enantiomorphic, Pyro / Piezo (p), Tetragonal, and Optical Activity. The 'Space Group' panel has a dropdown for Space Group Symbol. The 'Physical Properties' panel has a dropdown for Axis (Å) and a 'Convert Cell for Search...' button. The 'Author's Cell' panel has input fields for a, b, c, β , γ , and Volume. The 'Convert Cell' dialog box is open, showing 'Author's Crystal System' set to Tridlinic (Anorthic), 'Author's Lattice Centering' set to Primitive, and 'Cell Type' set to Crystal. The 'Convert' button is highlighted.

Convert Cell form used to convert Author's 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 cell.

Search Window

Supercell/Subcell

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

The screenshot shows the ICDD Search Window interface. The window is titled "Search" and contains several sections for filtering search results:

- Subfile:** A list of subfiles including "Custom PDF Set", "Alkaloid", and "Amino Acid, Peptide & Complex".
- Environment:** Checkboxes for "Ambient", "Press. (Non-ambient)", "Temp. (Non-ambient)", and "Press. & Temp. (Non-ambient)".
- Status:** Checkboxes for "Primary", "Alternate", and "Deleted".
- Quality Mark:** A list of quality marks including "Star", "Good", "Indexed", "Calculated", "Prototyping", "Minimal Acceptable", "Blank", and "Low-Precision".
- Database:** Checkboxes for "ICDD (00)", "ICSD (01)", "CSD (02)", "NIST (03)", "LPF (04)", and "ICDD Crystal Data (05)".
- Crystal (Symmetry Allowed):** Checkboxes for "Centrosymmetric" and "Non-centrosymmetric", with sub-options for "Enantiomorphic", "Pyro / Piezo (p)", "Optical Activity", and "Piezo (2nd Harm.)".
- Atomic Environment Type:** A table with columns for "Symbol" and "Elements".
- Space Group Symbol:** A dropdown menu.
- Crystal Data:** Input fields for "Axis (Å)" (a, b, c) and "ESD" (a, b, c, V).
- Supercell/Subcell:** Radio buttons for "Supercell" and "Subcell", and a "Volume Ratio" field set to "1" to "1".

At the bottom of the window, there are buttons for "Search", "Reset Tab", "Reset All", and "Help", along with a "Numeric Input" and "Global Operator" dropdown.

Search Window Modulated

Search

Subfile

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

Environment

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

Status

- Primary
- All
- De

Quality Mark

- Star
- Minimal Acceptable
- Blank
- Low-Precision

Database

- ICDD (00)
- ICDD Crystal Data (05)

Modulated Dimension

- 3 + 1d
- 3 + 2d
- 3 + 3d

Subsystems

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

Search

Reset Tab

Reset All

Help

Numeric Input

Global Operator

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

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

Search Window Diffraction

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

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
- Press. (Non-ambient)
- Temp. (Non-ambient)
- Press. & Temp. (Non-ambient)
- 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

Melting Point (K)

Value ESD

Density (g/cm³)

Value ESD

Measured Density Calculated Density Structural Density

Color

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

Property Sheet

Search Reset Tab Reset All Help Numeric 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 Window interface showing the References section. The interface includes a left sidebar with a tree view of categories (e.g., Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial) and a right sidebar with environmental filters (Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, Raw Diffraction Data). The main search area contains fields for DOI, Title, Author, Publication (set to Journal/Patent), Volume, and Year (Start Year, End Year). A red box highlights the search filters, and a red arrow points to the Publication dropdown menu.

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

The screenshot displays the ICDD Search Window interface. At the top, there are several filter sections: 'Subfile' (set to Custom PDF Set), 'Environment' (with checkboxes for Ambient, Press. (Non-ambient), Temp. (Non-ambient), Press. & Temp. (Non-ambient), Atomic Coordinates, and Raw Diffraction Data), 'Status' (with checkboxes for Primary, Alternate, and Deleted), 'Quality Mark' (with radio buttons for Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, and Low-Precision), and 'Database' (with checkboxes for ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), and ICDD Crystal Data (05)).

On the left side, there is a 'Periodic Table' and a list of search criteria: Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The 'Comments' criterion is currently selected.

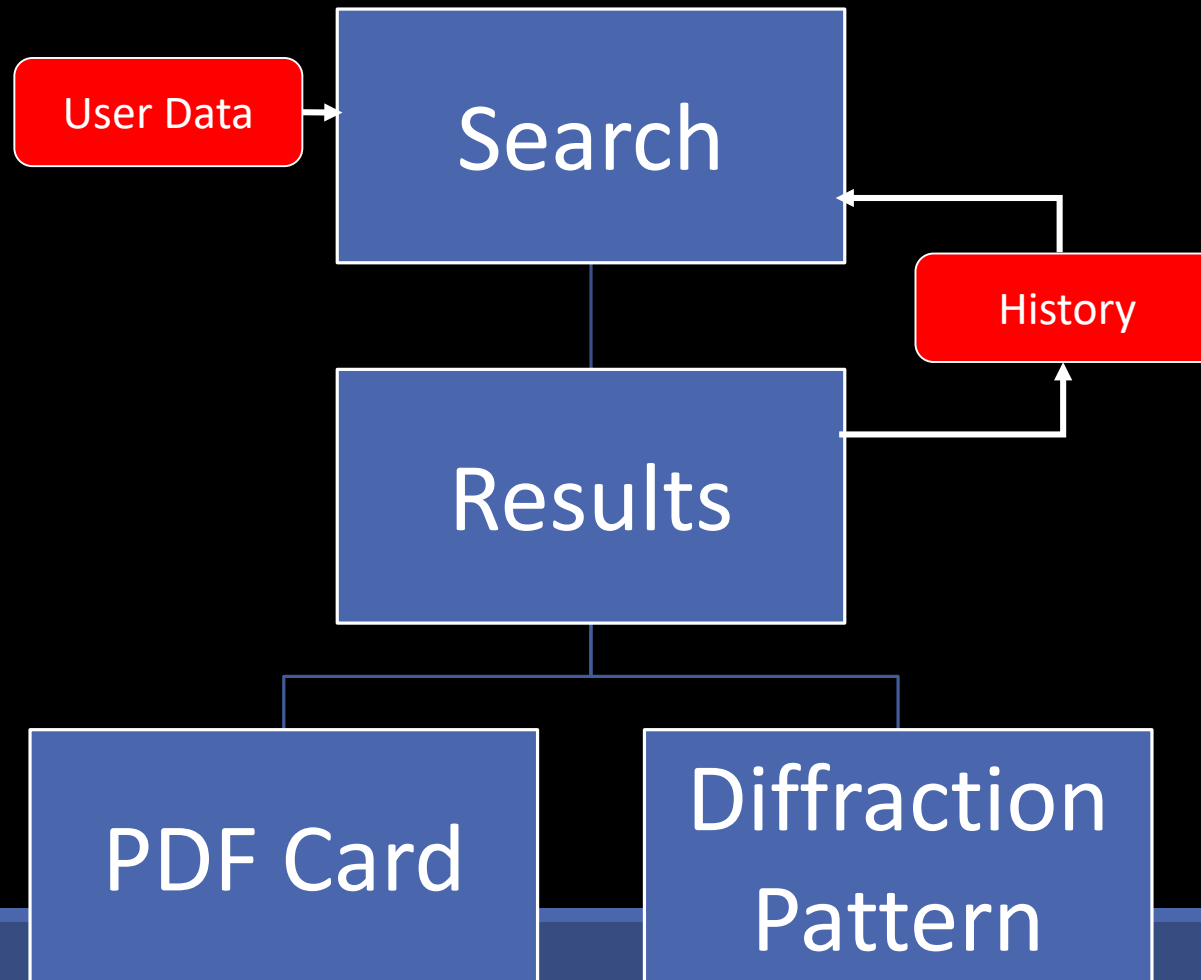
The main search area is titled 'Database Comments' and contains a search input field. Below it is a list of search results, including: Absolute Configuration, Additional Diffraction Lines, Additional Patterns, Analysis, ANX, Atomic Position, Bioactivity, Boiling Point, and Calculated Pattern Original Remarks. A red box highlights the search input field with the text: "Filter based on the text contained in comments."

At the bottom of the window, there are buttons for 'Search', 'Reset Tab', 'Reset All', and 'Help', along with a 'Numeric Input' dropdown and a 'Global Operator' dropdown.

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

Select Space Group

Select Compound Name

Selected filters highlighted in red

Search Results

Choose fields to be displayed in results

Results - 9 of 398,726

File Fields Set: My Defaults Tools Help

PDF #	QM	Chemical Formula	Search Results	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Coords
00-009-0367	I	$K_2 Pt Cl_4$	Pota	6.940000	3.160000	3.550000	T	✓
01-073-1506	I	$K_2 (Pt Cl_4)$	Potassium Platinum Chloride	6.990000	3.169250	3.555730	T	✓
04-006-6128	P	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	✓
04-007-2797	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.023000	3.183810	3.571940	T	✓
04-007-5356	I	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.025000	3.182100	3.569270	T	✓
04-007-7303	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	6.996100	3.159080	3.540590	T	✓
04-007-7304	S	$K_2 Pt Cl_4$	Potassium Platinum Chloride	6.981300	3.156210	3.538480	T	✓
04-009-8290	B	$K_2 Pt Cl_4$	Potassium Platinum Chloride	7.024000	3.183270	3.571050	T	✓
04-013-8855	B	$K_2 Pt (CN)_4 Cl_{0.32} (H_2 O)_{2.6}$	Potassium Platinum Chloride Cyanid...	9.866000	4.412210	6.976320	T	✓

[(Pt And Cl)] And [Any Name Contains Fragments 'Potassium' And 'Platinum' And 'Chloride'] And [Space Group Symbol Contains Phrase 'P4/mmm'] And [Status (Primary, Alternate)]

Search Filters

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



Preferences Module

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

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

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

Other X-ray... 1.540598 0 Simulated Profile (Calc)

Fixed Slit Intensity Raw Diffraction Data

2θ (°)	d (Å)	I	h	k	l	*
12.594	7.023000	999	1	0	0	
17.847	4.966010	103	1	1	0	
21.401	4.148600	233	0	0	1	
24.908	3.571940	398	1	0	1	
25.343	3.511500	66	2	0	0	
28.002	3.183810	530	1	1	1	

Intensity vs. 2θ (°) plot showing experimental data (red) and simulated profile (black).

PDF Status: Primary Quality Mark: ● Star Pressure/Temperature: Ambient Temperature: 297.0 K

Phase: -

Chemical Formula: K_2PtCl_4

Structural Formula: -

Empirical Formula: Cl_4K_2Pt

Weight %: Cl34.16 K18.84 Pt47.00

Atomic %: Cl57.14 K28.57 Pt14.29

Compound Name: Potassium Platinum Chloride

Mineral Name: - IMA No: -

Alternate Name: potassium tetrachloroplatinate(II)

CAS Number: -

Entry Date: 09/01/2005

Last Modification Date: 09/01/2011 Last Modifications: Reflections

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.

The screenshot displays the ICDD software interface. At the top, a header indicates 'Results - 9 of 398,726'. Below this is a table of PDF entries:

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

A context menu is open over the row with PDF # 04-007-7303, showing options: 'Open PDF Card', 'Add to Custom PDF Set...', 'Remove from Custom PDF Set...', 'Tools/Simulations', 'Copy PDF #', 'Select All', and 'Remove Rows'. Below the table, a filter is shown: '[[Pt And Cl]] And [Any Name Alternate]]'. To the right, three windows are open, each displaying a PDF data card for a different PDF #. The most prominent window is for PDF # 00-009-0367, which includes a diffraction pattern plot and a table of diffraction data:

2θ (°)	d (Å)	I	h	k	l	*
12.745	6.940000	100	1	0	0	
17.978	4.930000	15	1	1	0	
21.552	4.120000	30	0	0	1	
25.064	3.550000	50	1	0	1	
25.502	3.490000	5	2	0	0	
28.218	3.160000	65	1	1	1	

The data card also shows a 'PDF' section with the following details:

- Status: Primary
- Quality Mark: Indexed
- Pressure/Temperature: Ambient
- Temperature: 298.0 K
- Phase: -
- Chemical Formula: K_2PtCl_4
- Structural Formula: -
- Empirical Formula: Cl_4K_2Pt
- Weight %: Cl34.16 K18.84 Pt47.00
- Atomic %: Cl57.14 K28.57 Pt14.29
- Compound Name: Potassium Platinum Chloride
- Mineral Name: - IMA No: -
- Alternate Name: -
- CAS Number: 10025-99-7
- Entry Date: 09/01/1959
- Last Modification Date: - Last Modifications: -

PDF Data Card Features

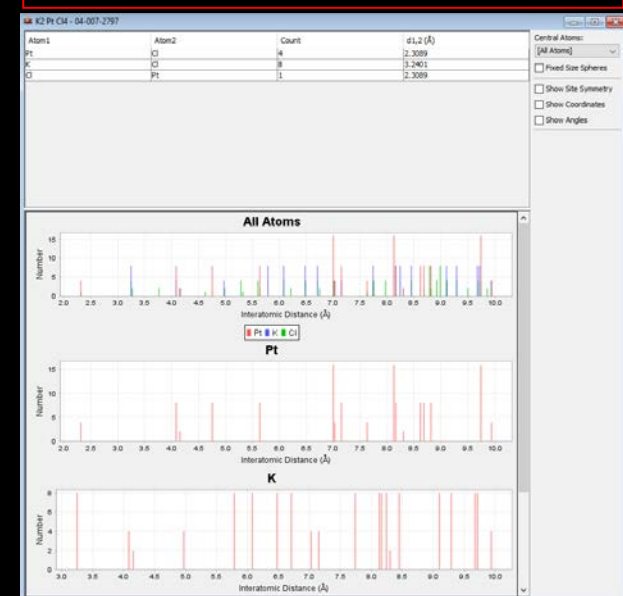


View Temperature Series

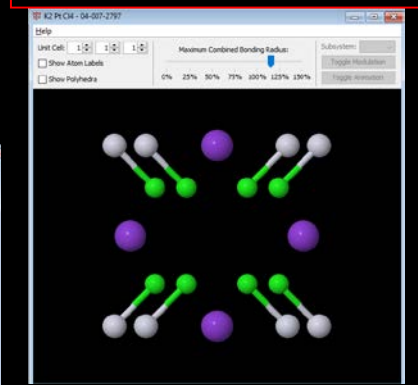
Temperature Series (K2 Pt Cl4 - 04-007-2797)

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

View Bond Distances/Angles



View 3D Structure



View Toolbox

Toolbox

Author's Cell Parameters

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

α (°): 90 β (°): 90 γ (°): 90

Edit Cell Parameters

Wavelength (Å): 1.540598

Peak Planar Angles Reflections

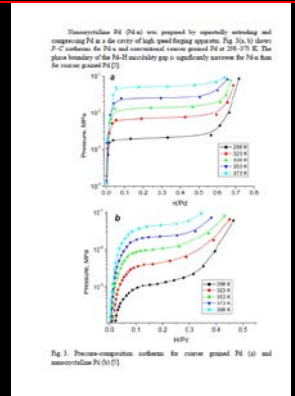
Miller Index Results

h: 0 d: 4.149 Å

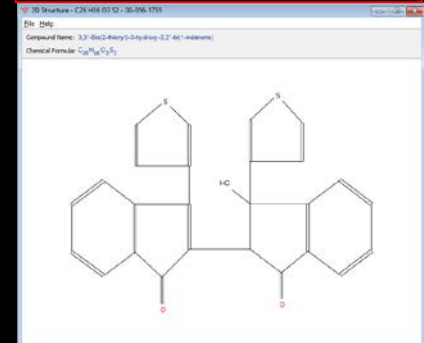
k: 0 2θ: 21.401°

l: 1

View Property Sheet



View 2D Structure

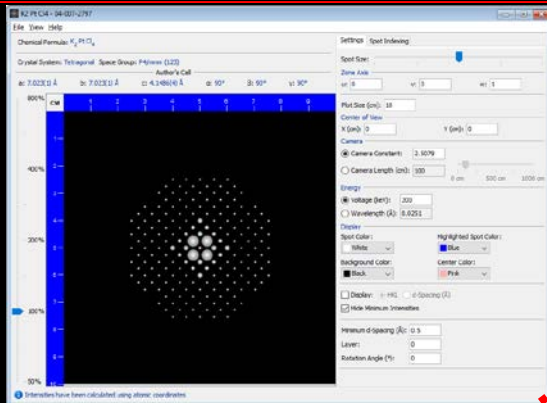


Note: The availability of each feature varies by PDF entry.

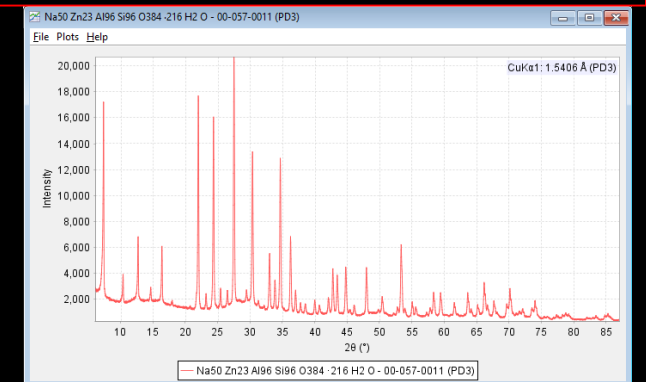
PDF Data Card Features



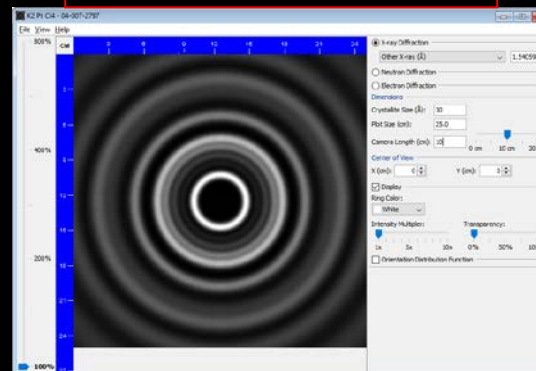
View Simulated Electron Spot Pattern



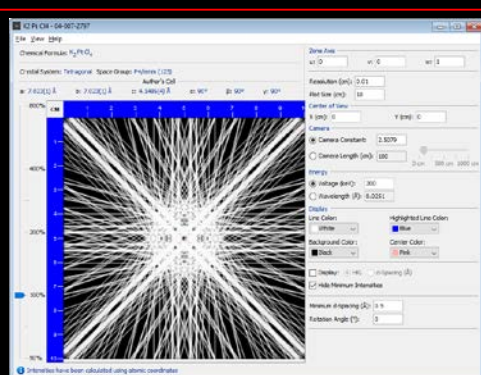
View Raw Diffraction Data (PD3)



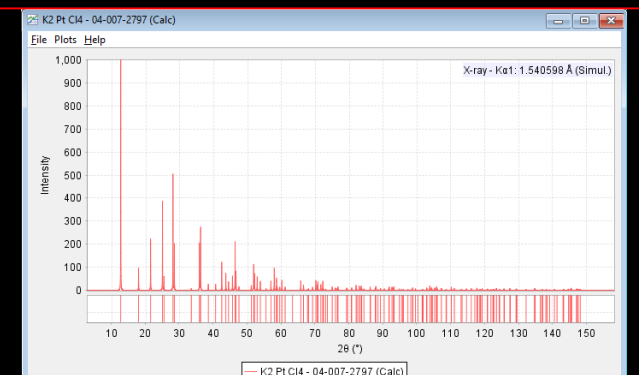
View Ring Pattern



View Electron Backscattering Pattern



View Simulated Diffraction Profile





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