PDF-4+ Tools and Searches

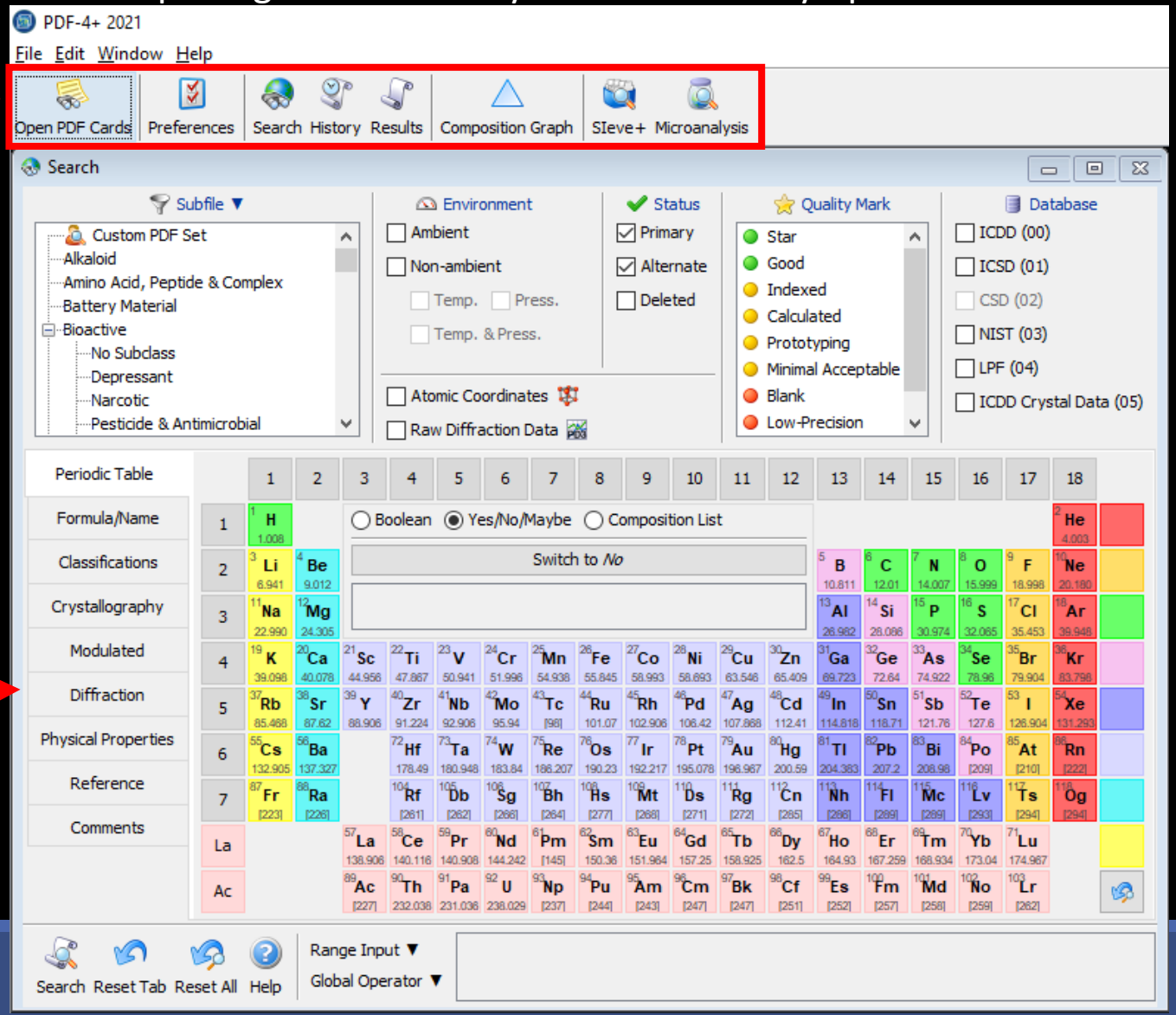
PDF-4+ 2021

The PDF-4+ 2021 database is powered by our integrated search display software. PDF-4+ 2021 boasts 77 search selections coupled with 131 display fields resulting in a nearly limitless choice of data mining options. This quick tutorial will introduce you to the basics of PDF-4+ filters available to you to refine your search.

- Getting Started: The Toolbar
- Search Window: Overview of Search Classifications
- Data Mining Basics
- Search Example
- Preferences Module
- PDF Data Card

Launch Screen

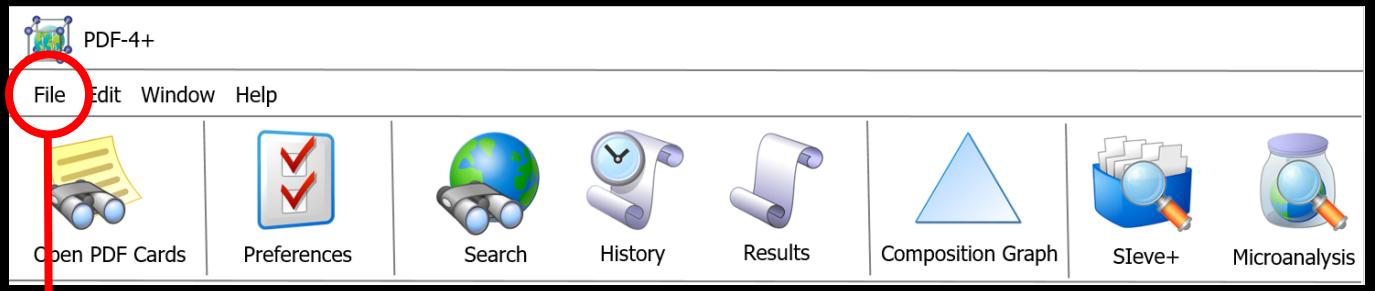
This will be the opening screen when you have correctly opened PDF-4+ 2021.

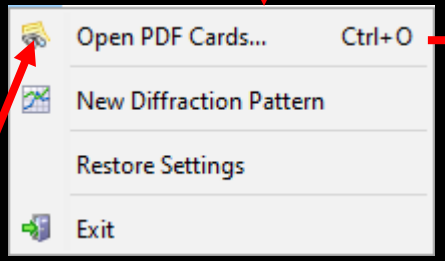


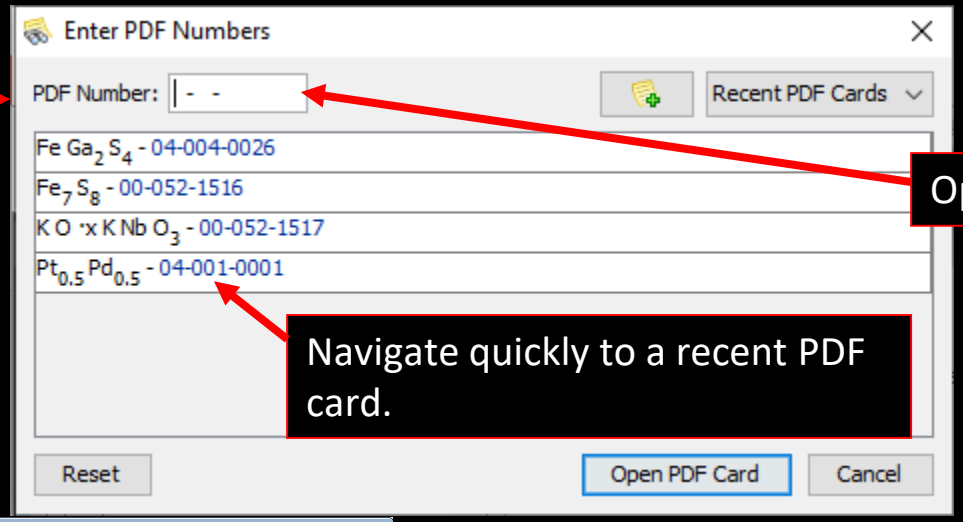
Tool Bar

Primary Search Menu

Getting Started



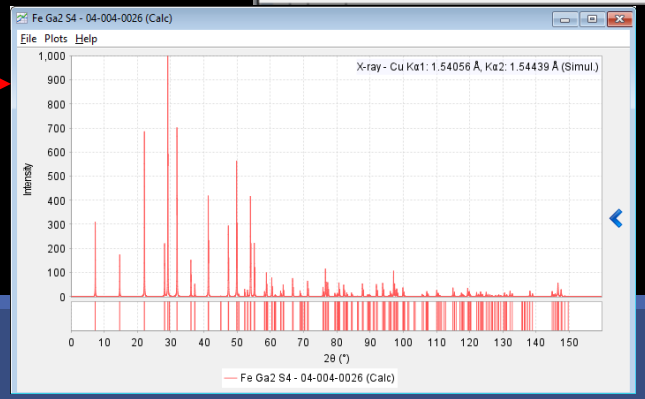




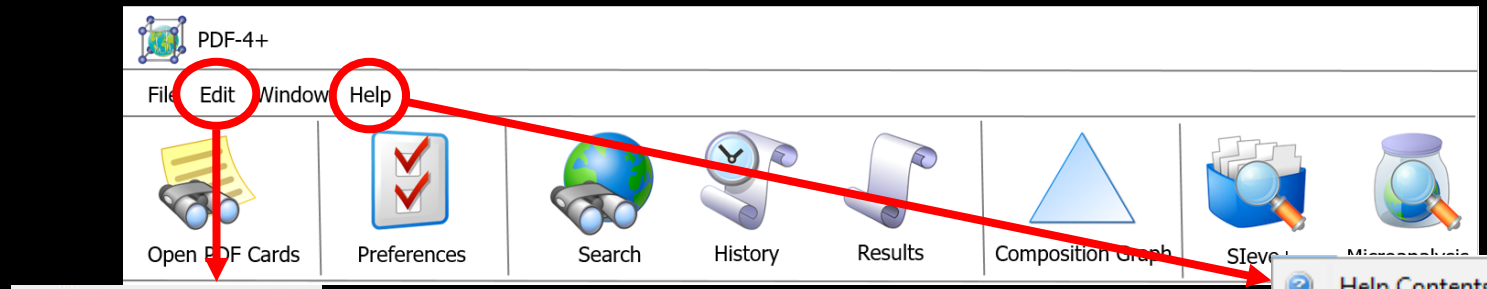
Open a known PDF card.

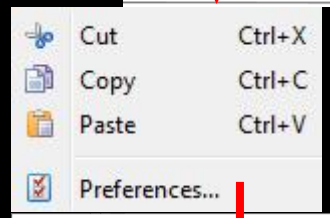
Navigate quickly to a recent PDF card.

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

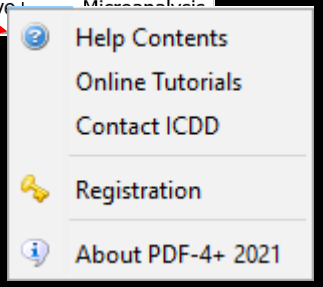


Getting Started

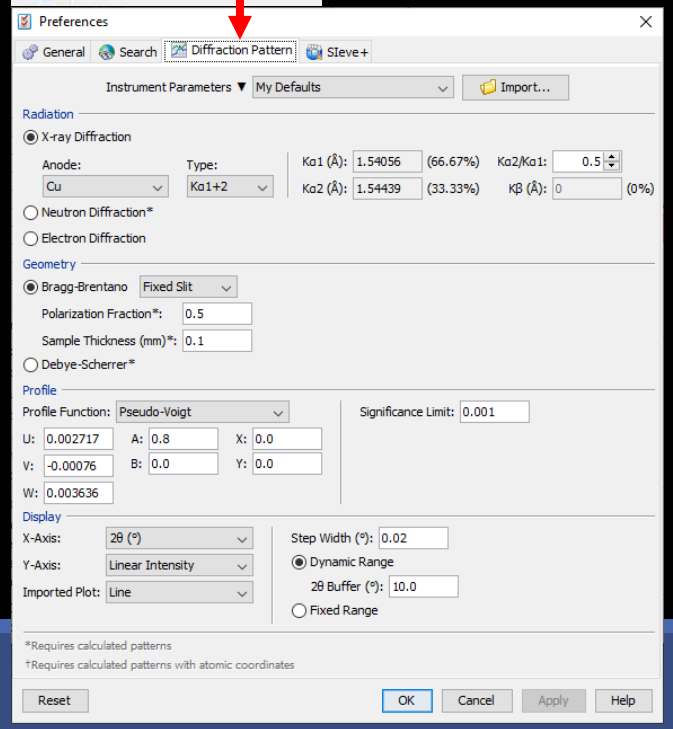




Edit functions

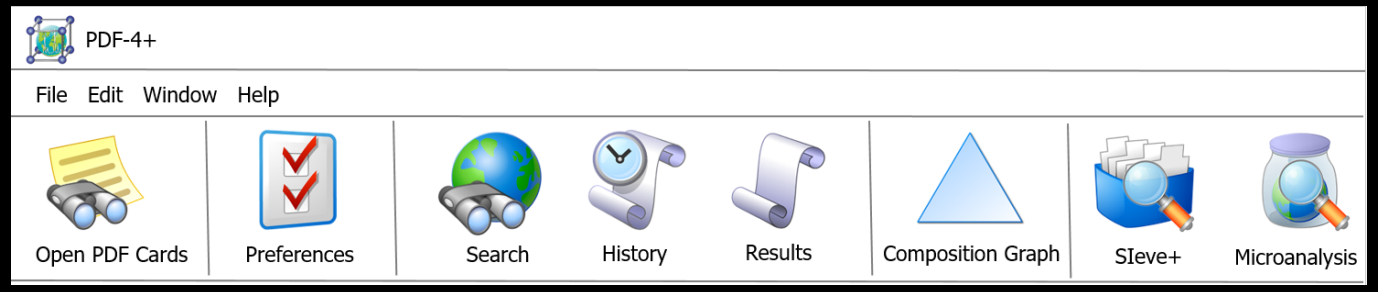


Help information regarding use, support, license policy, and registration of the PDF-4+.



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

Tool Bar



Quick Navigation Icons


Select a PDF Card


Select Preferences Module


Open Search Window


Open History Window


Open Results Window

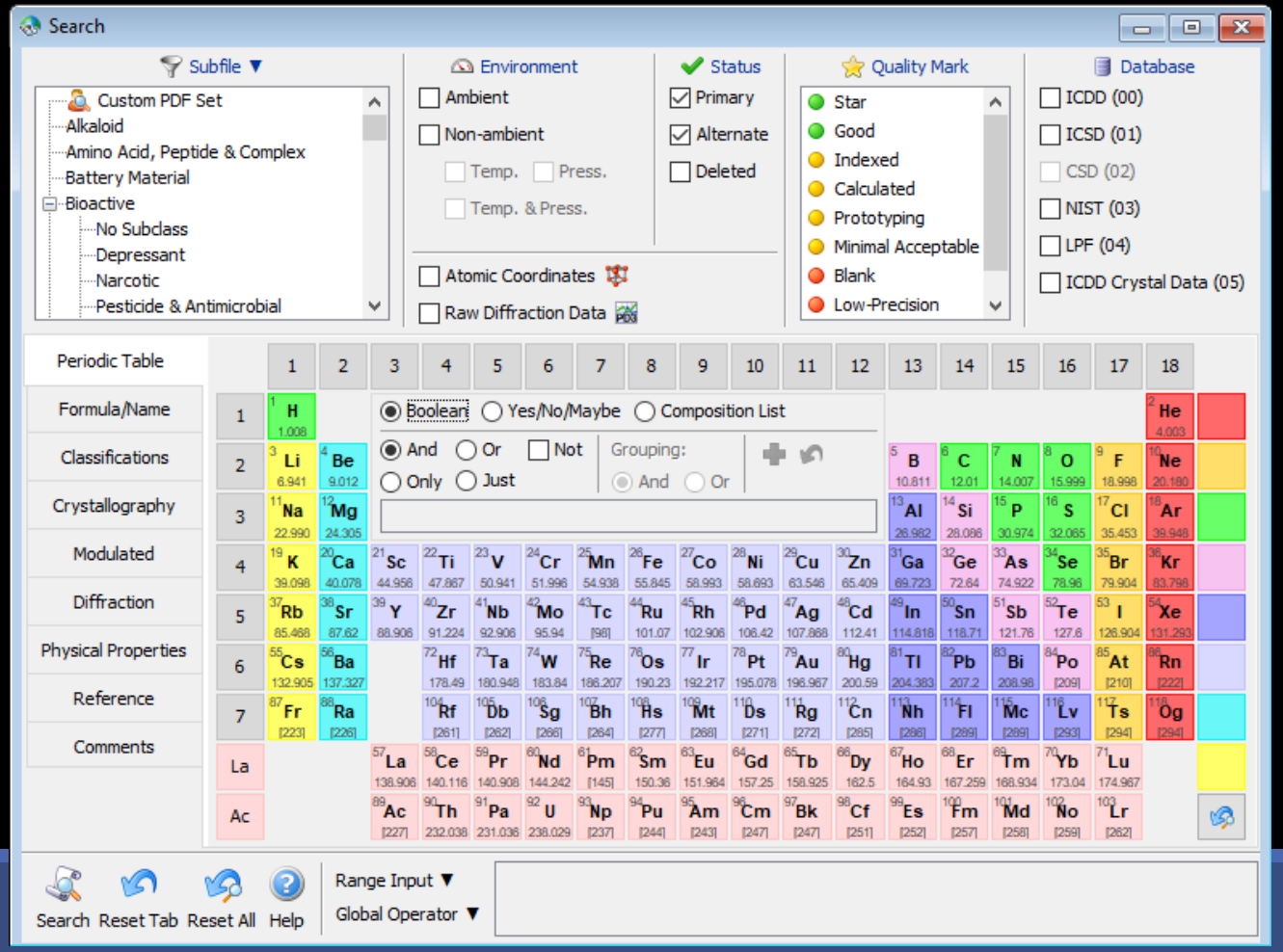

Composition Graph


Open Sleve+

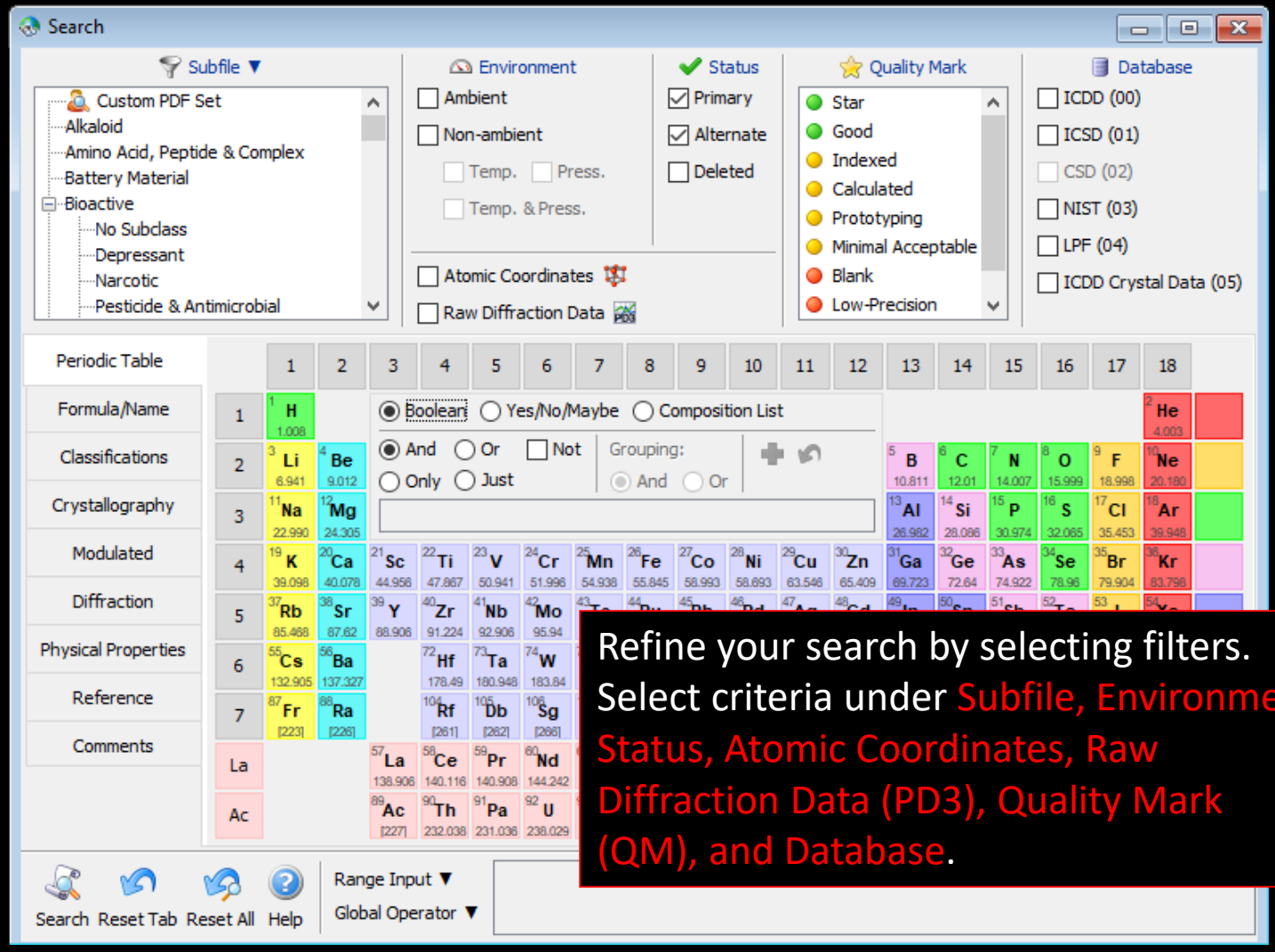

Microanalysis

Primary Search Menu

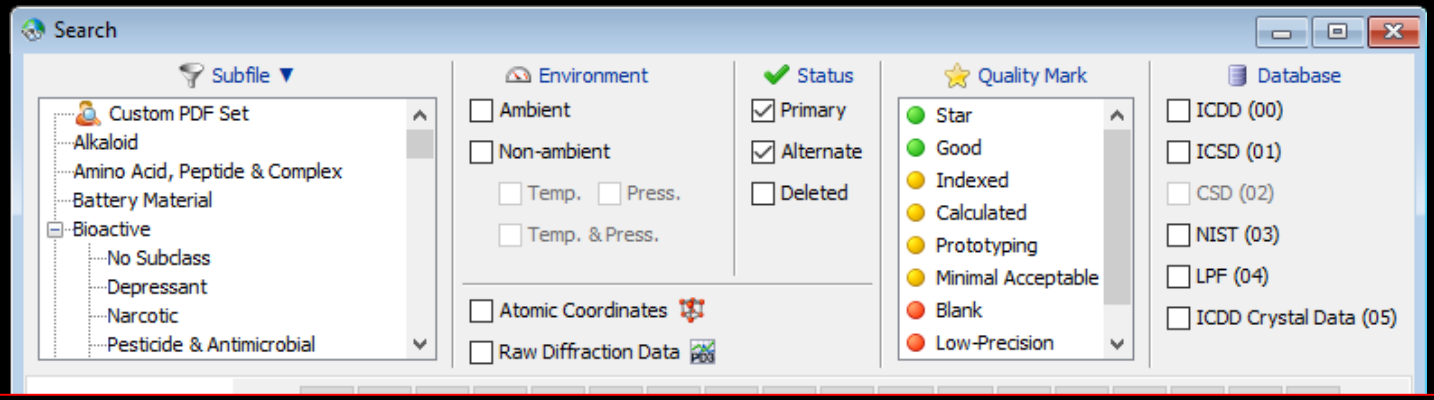
The Search Window displays nine tabs. Each tab features multiple search criteria to allow you to data mine the PDF-4+. Searching the PDF-4+ is an iterative process that allows you to input user-defined criteria, view the results, and combine additional criteria to refine your results.



Search Window
Subfiles/Database Filters



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.

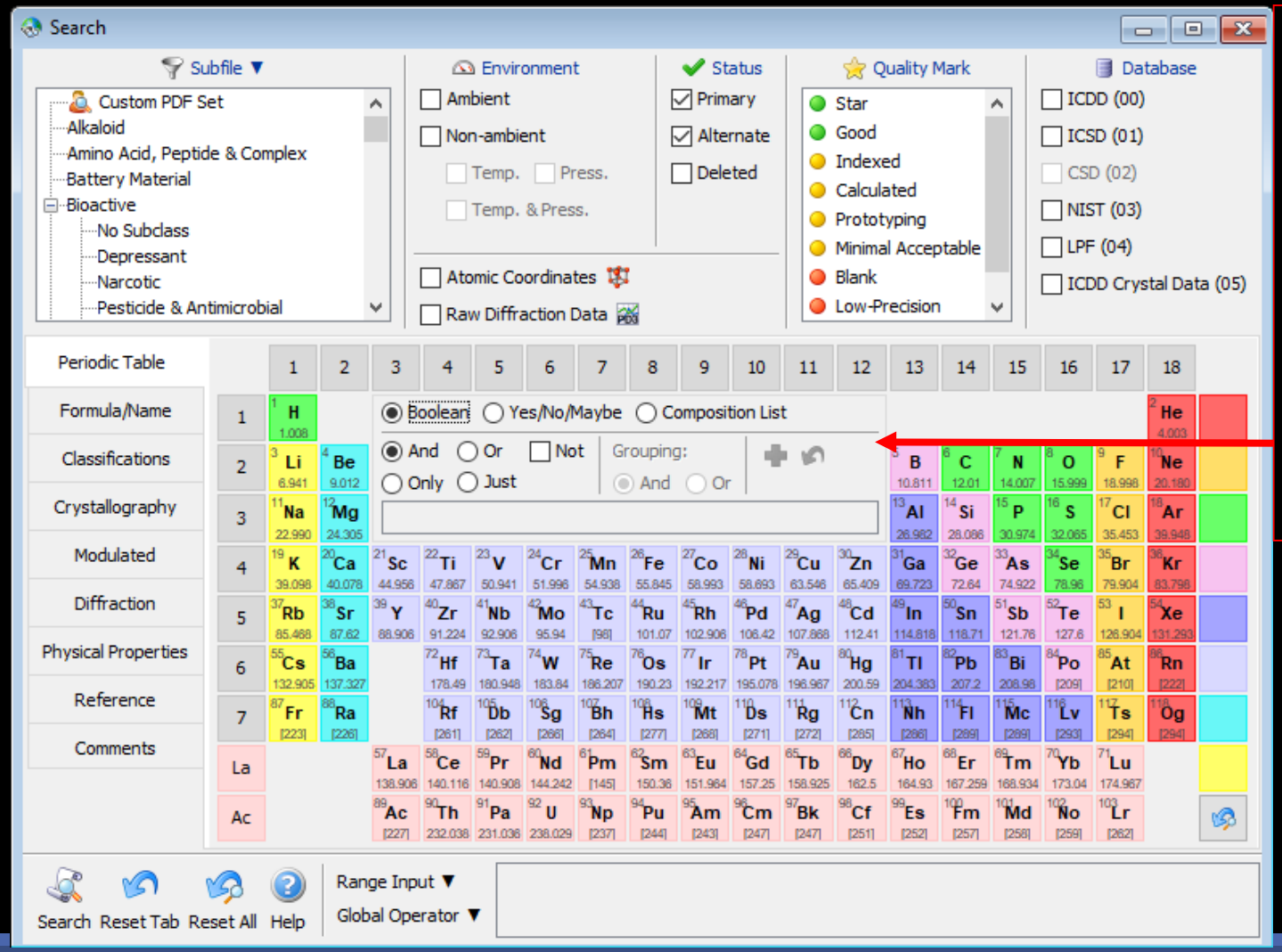
Status – select filters based on the status of the pattern, which can be Active, Deleted, Alternate, Rejected or Primary.

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



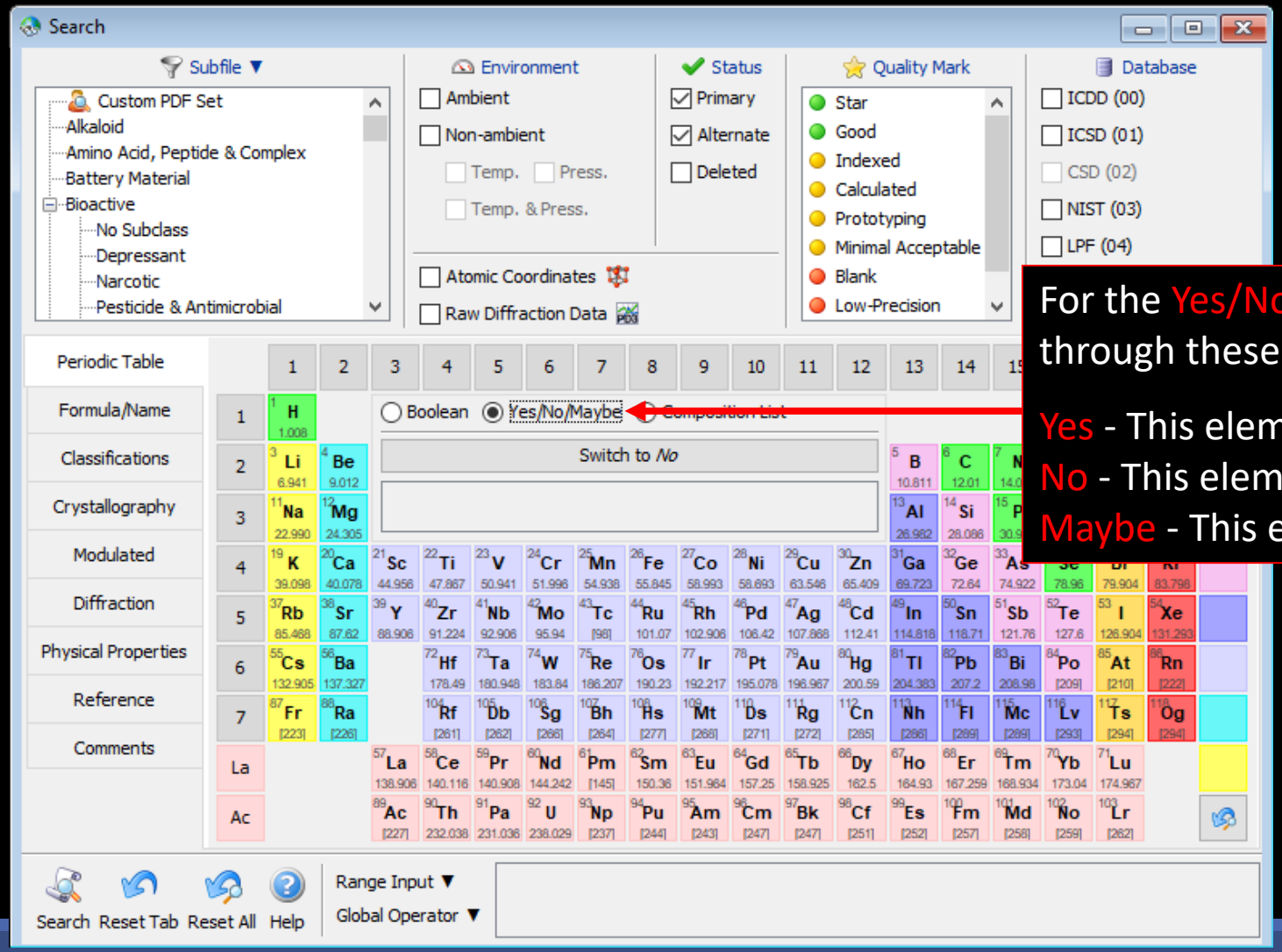
Refine your search by selecting filters based upon the elements in a material. Select elements individually (i.e., *H, He, Li*, etc.) or by group (i.e., *IA, Noble Gases, Period 1*, etc.).

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



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

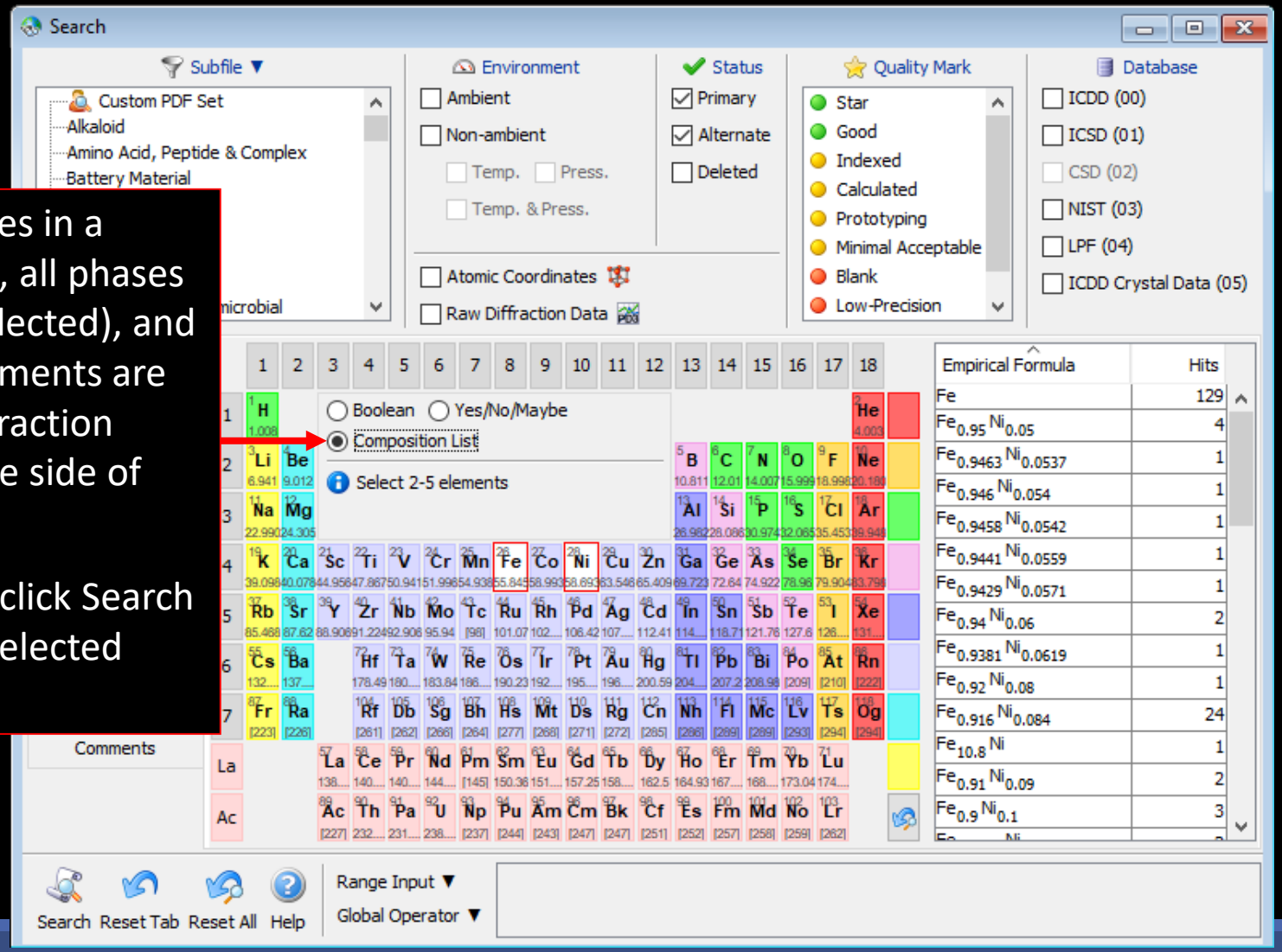
Yes - This element must exist in the pattern (white)
No - This element must not exist in the pattern (black)
Maybe - This element may exist in the pattern (colored)

Search Window

Periodic Table Filters

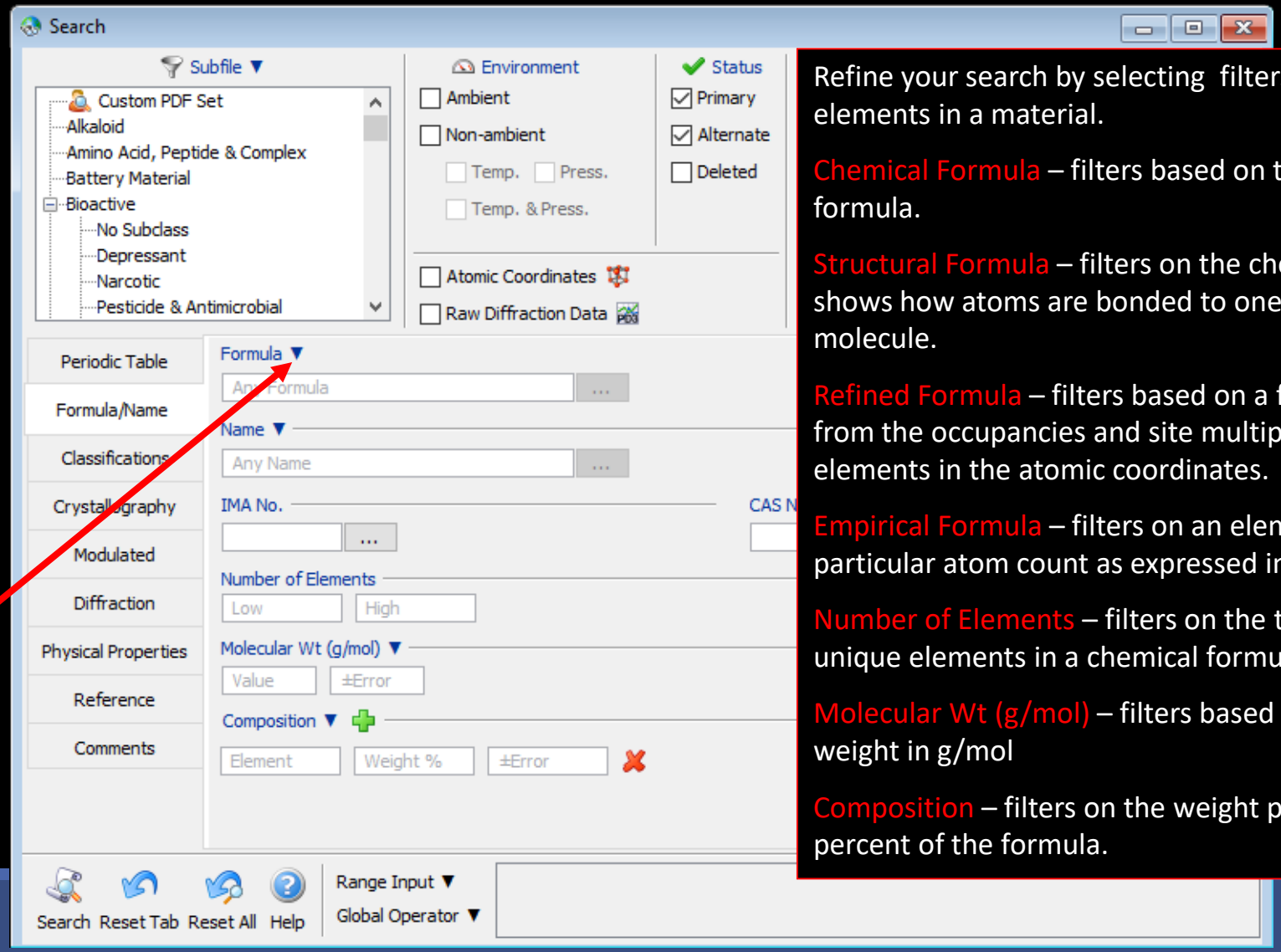
Composition Diagram List - This lists all phases in a binary system (if two elements are selected), all phases in a ternary system (if three elements are selected), and all phases in a quaternary system (if four elements are selected). The phases are sorted by atomic fraction (using the empirical formula),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

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



Search Window

Formula/Name



- Any Formula
- Chemical Formula
- Structural Formula
- Empirical Formula
- Refined Formula

- Contains Elements
- Contains Phrase
- Exactly

- Not

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

Chemical Formula – filters based on the molecular formula.

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

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

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

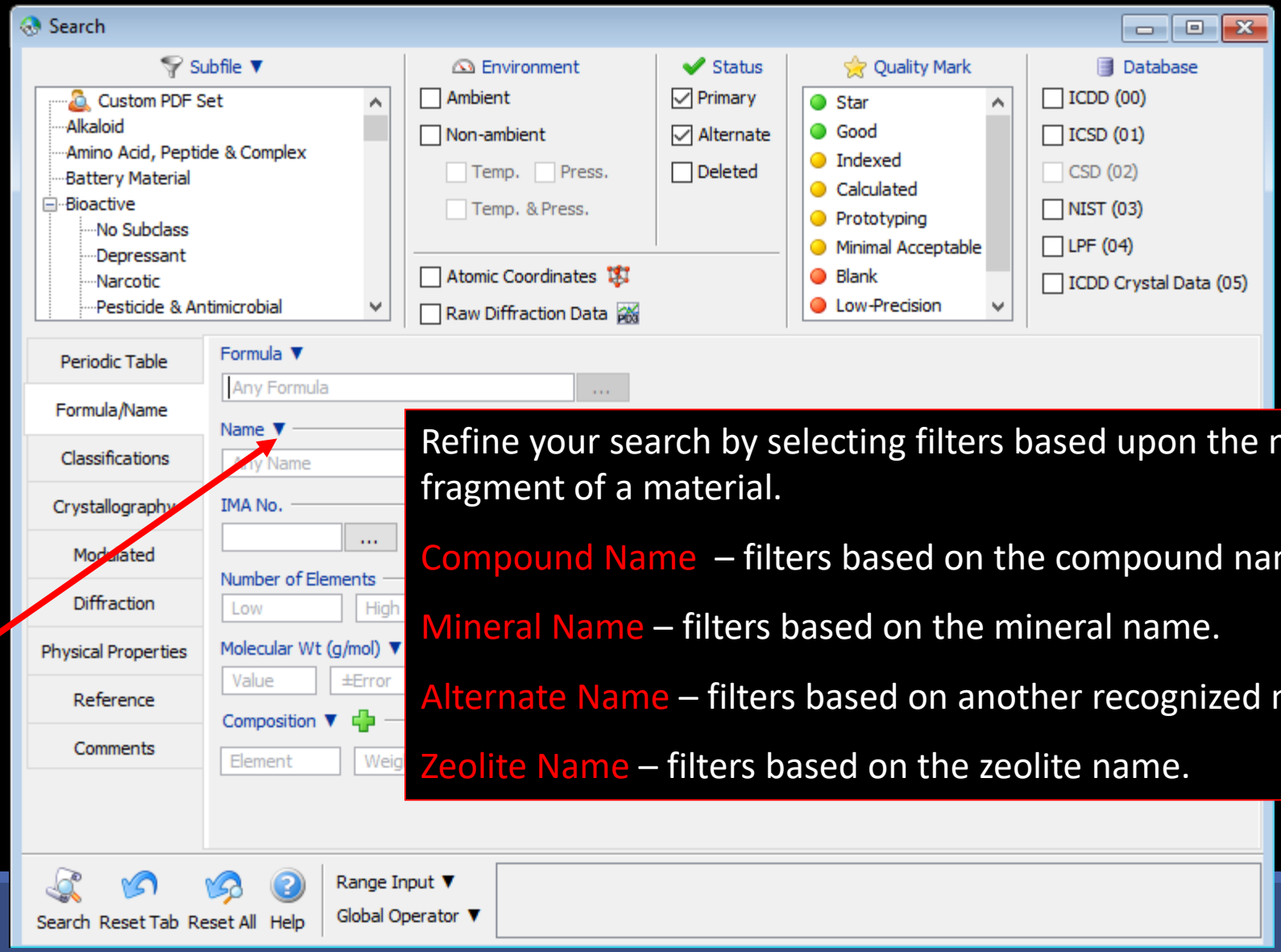
Number of Elements – filters on the total number of unique elements in a chemical formula.

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

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

Search Window

Formula/Name



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

Compound Name – filters based on the compound name.

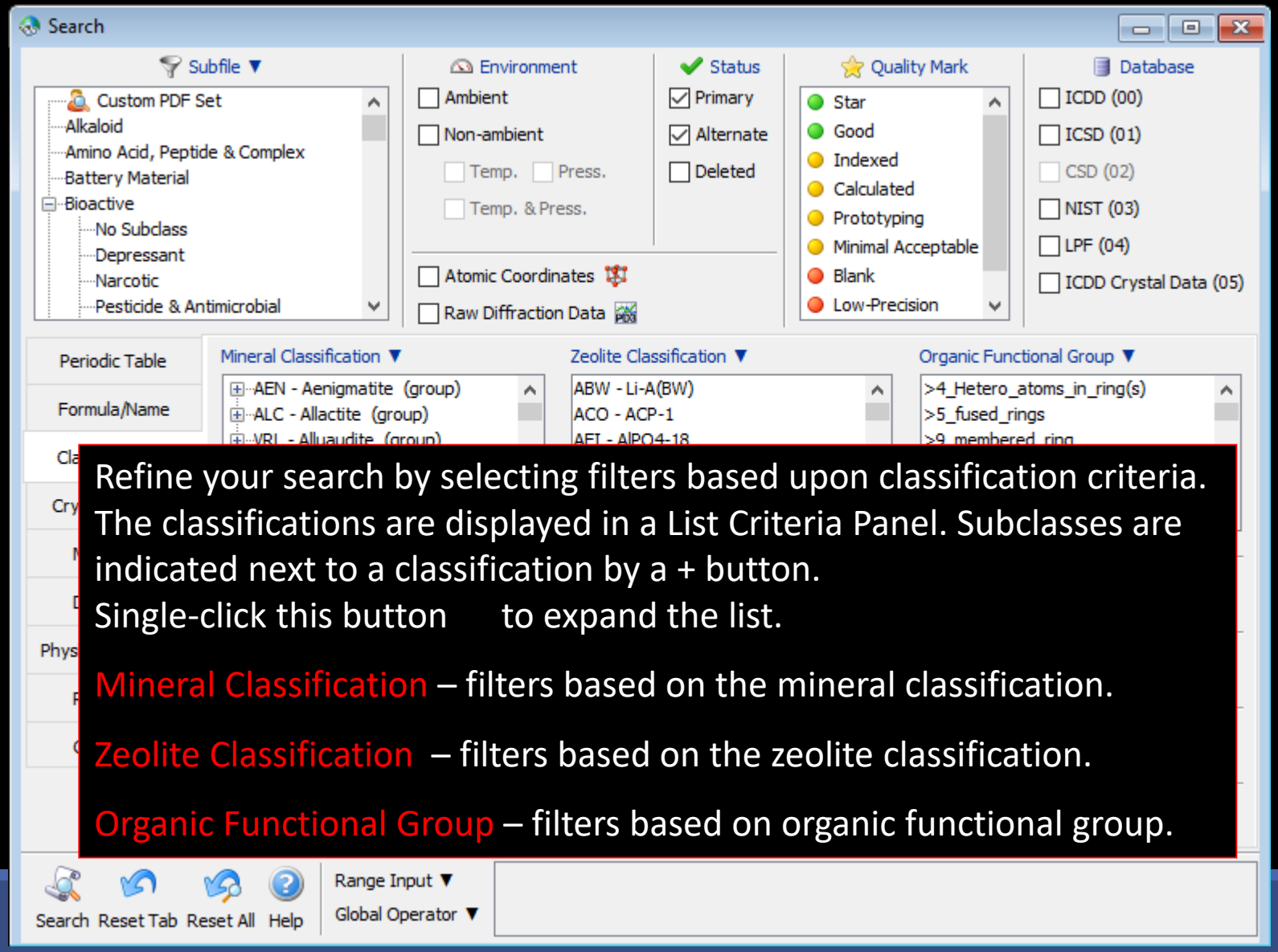
Mineral Name – filters based on the mineral name.

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

Zeolite Name – filters based on the zeolite name.

Search Window

Classifications



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.

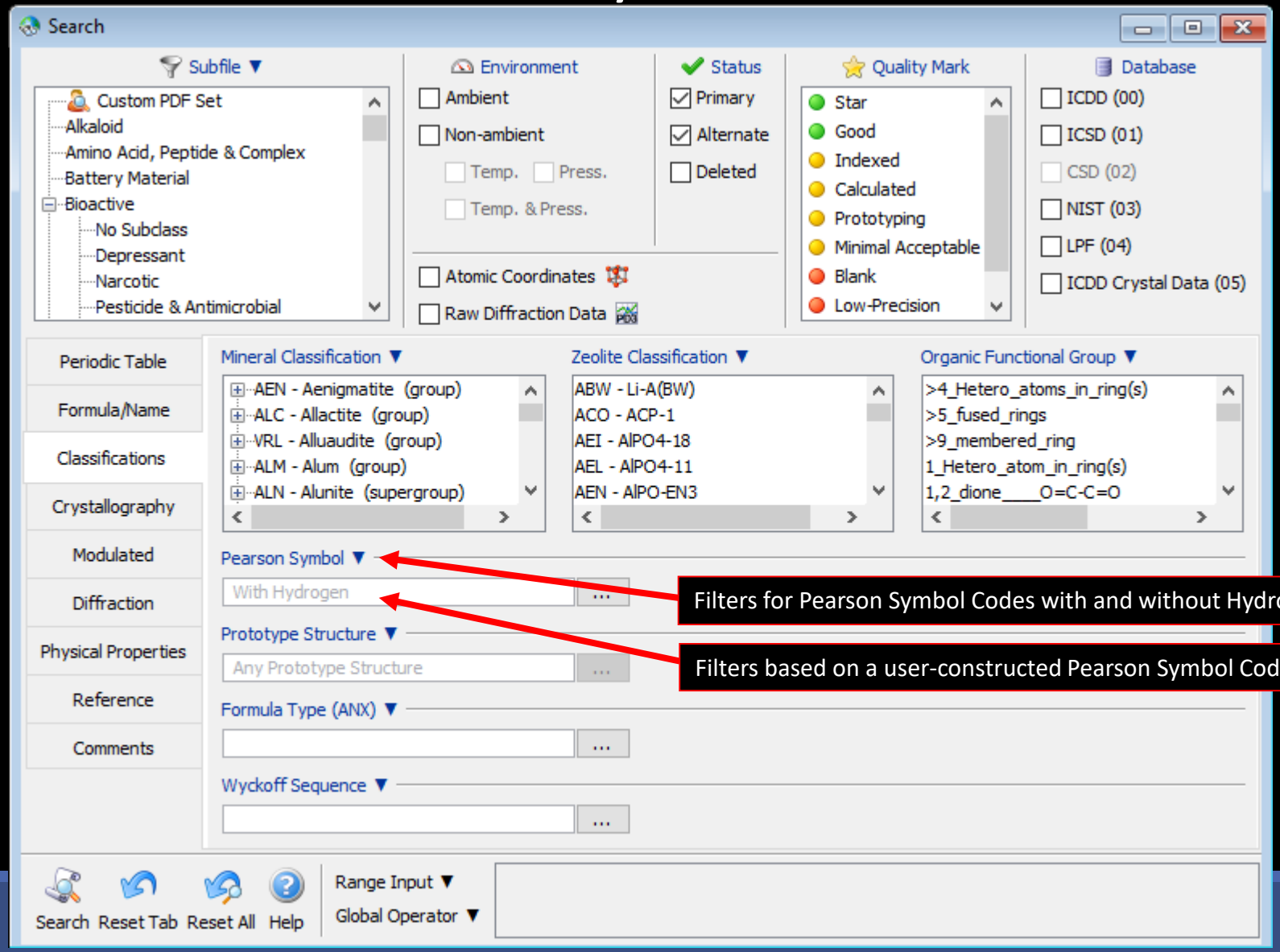
Mineral Classification – filters based on the mineral classification.

Zeolite Classification – filters based on the zeolite classification.

Organic Functional Group – filters based on organic functional group.

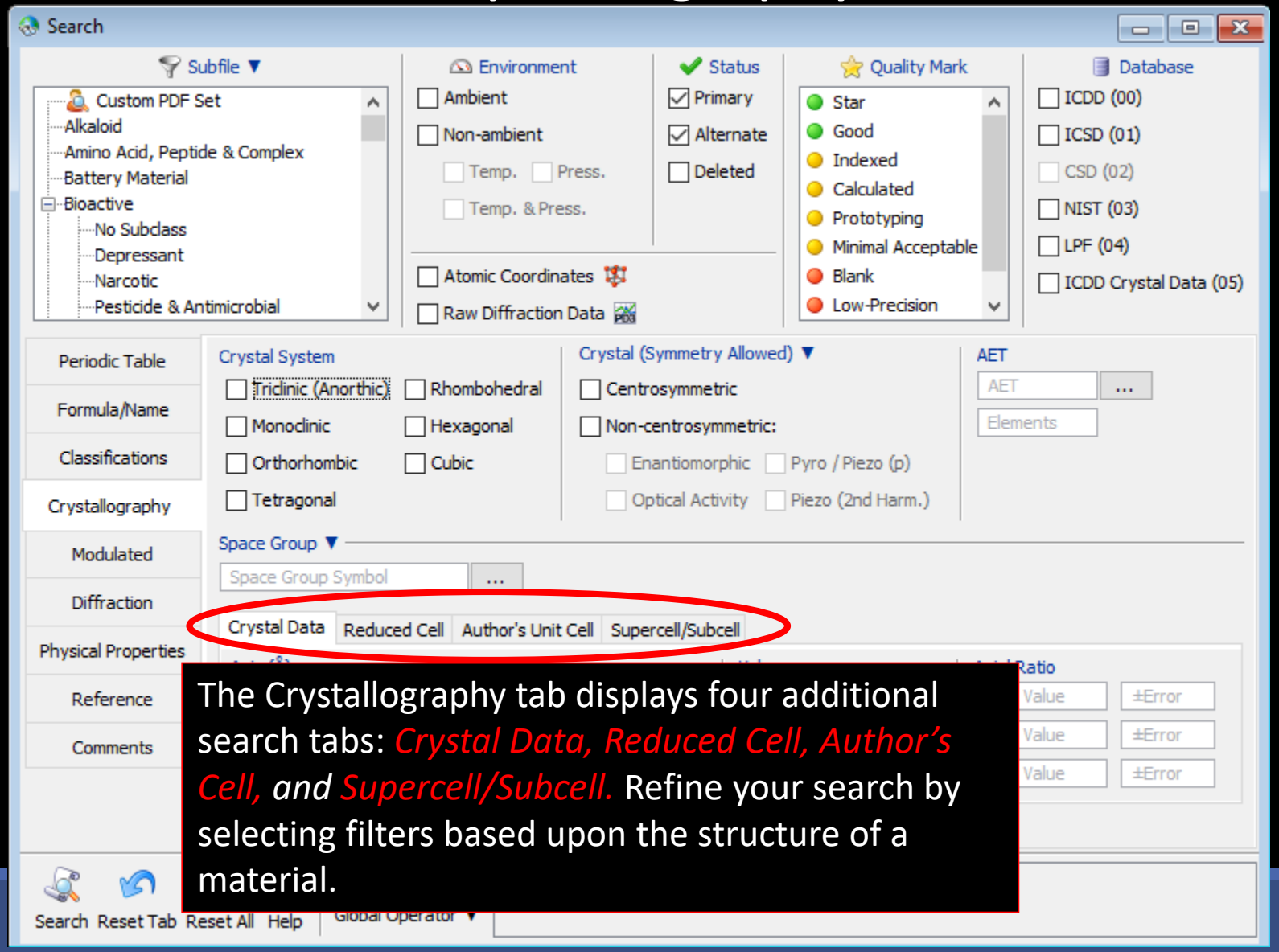
Search Window

Pearson Symbol Code



Search Window

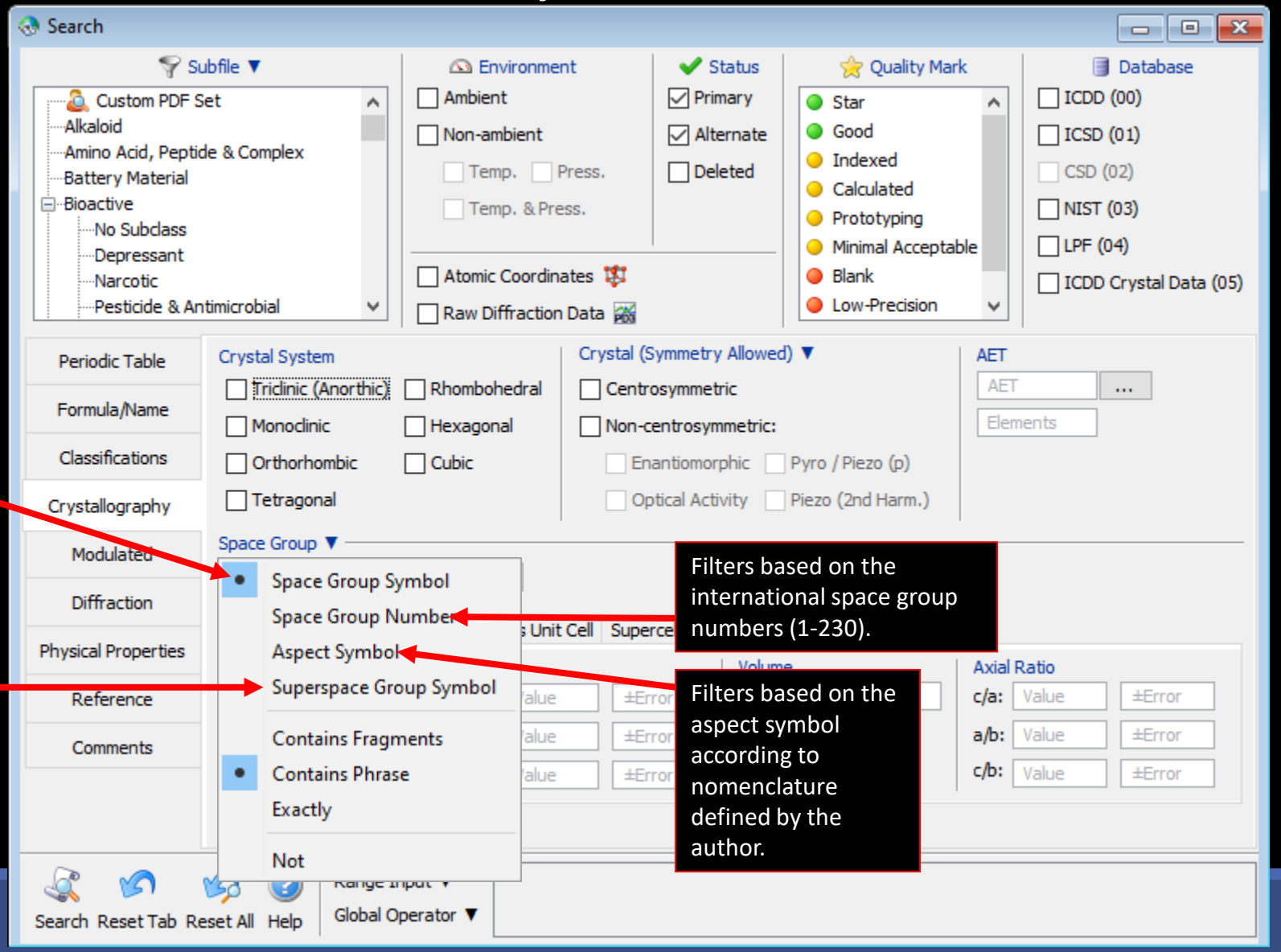
Crystallography



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



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

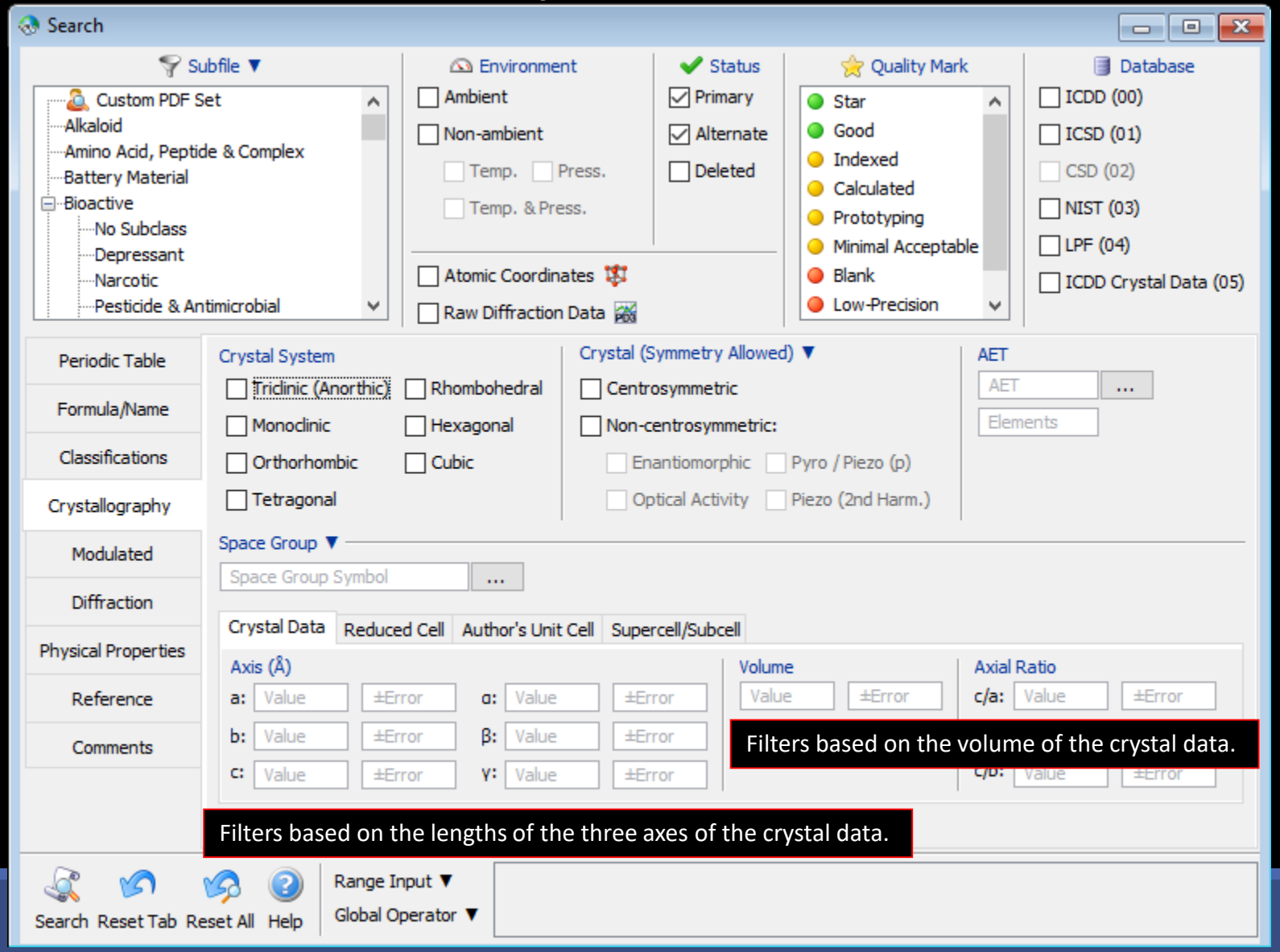
Filters based on the superspace group symbol (for modulated structures only).

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

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

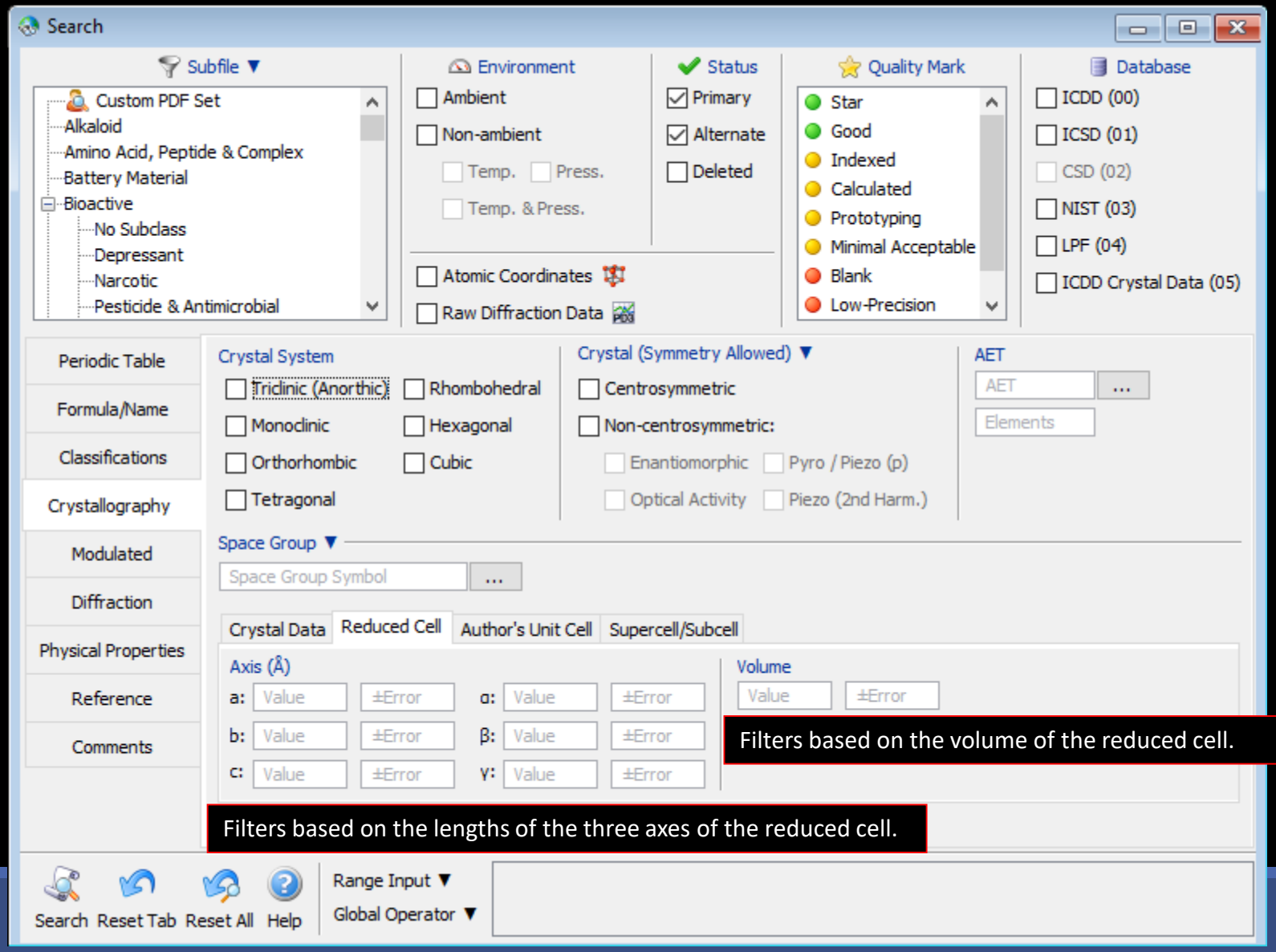
Search Window

Crystal Data



Search Window

Reduced Cell



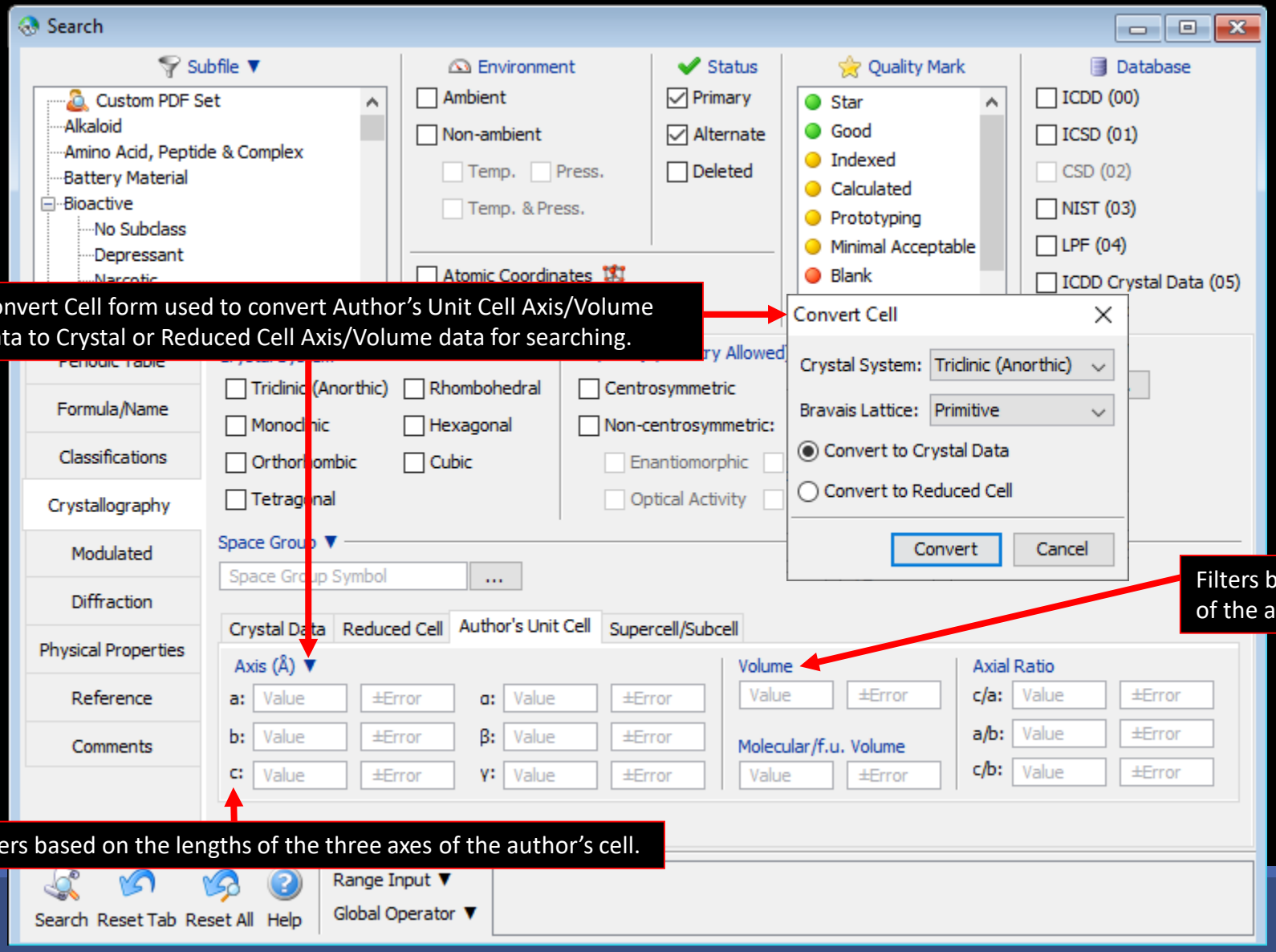
The reduced cell is a unique, primitive cell based on the three shortest lattice translations.

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



Convert Cell form used to convert Author's Unit Cell Axis/Volume data to Crystal or Reduced Cell Axis/Volume data for searching.

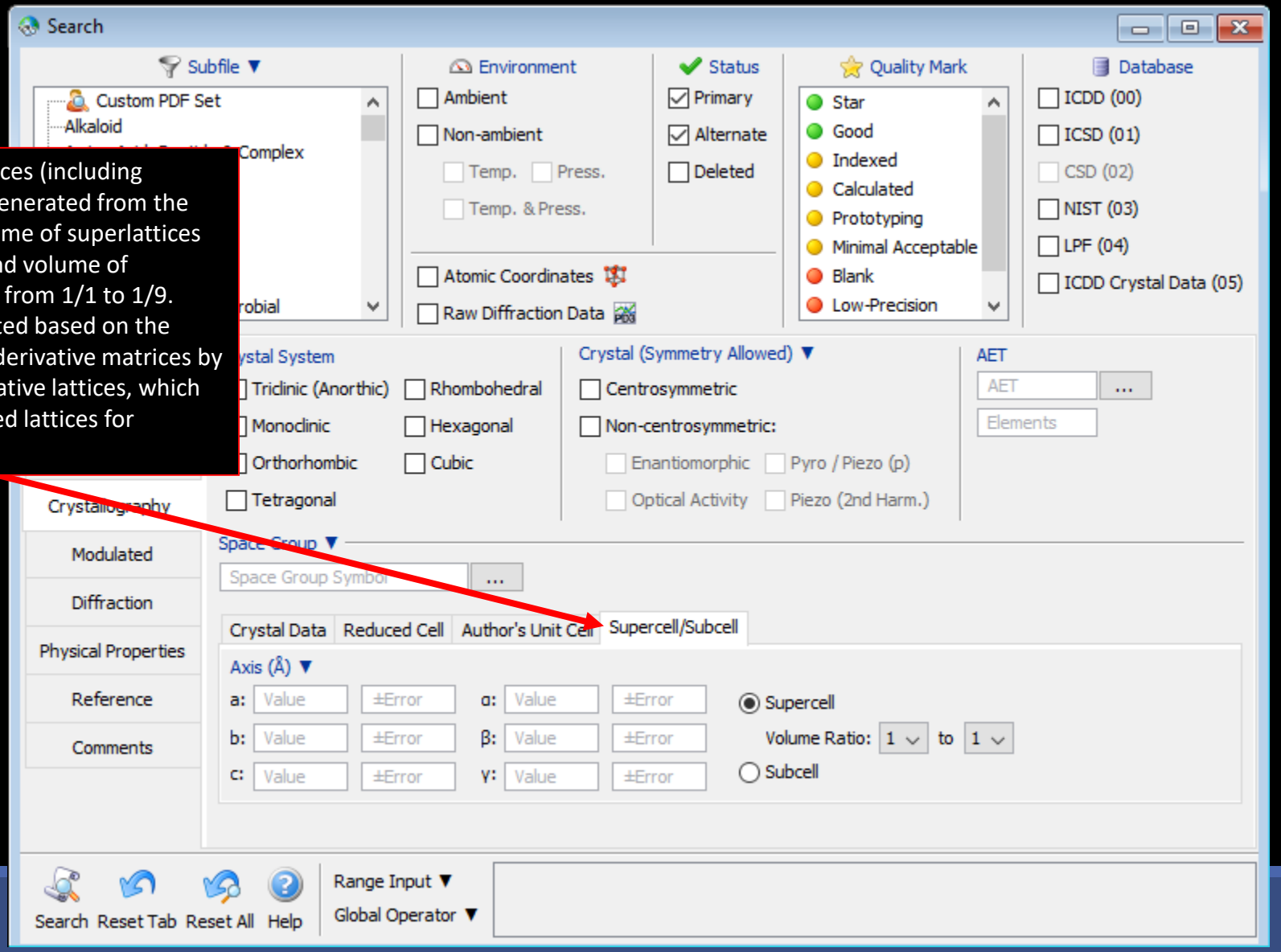
Filters based on the volume of the author's unit cell.

Filters based on the lengths of the three axes of the author's cell.

Search Window

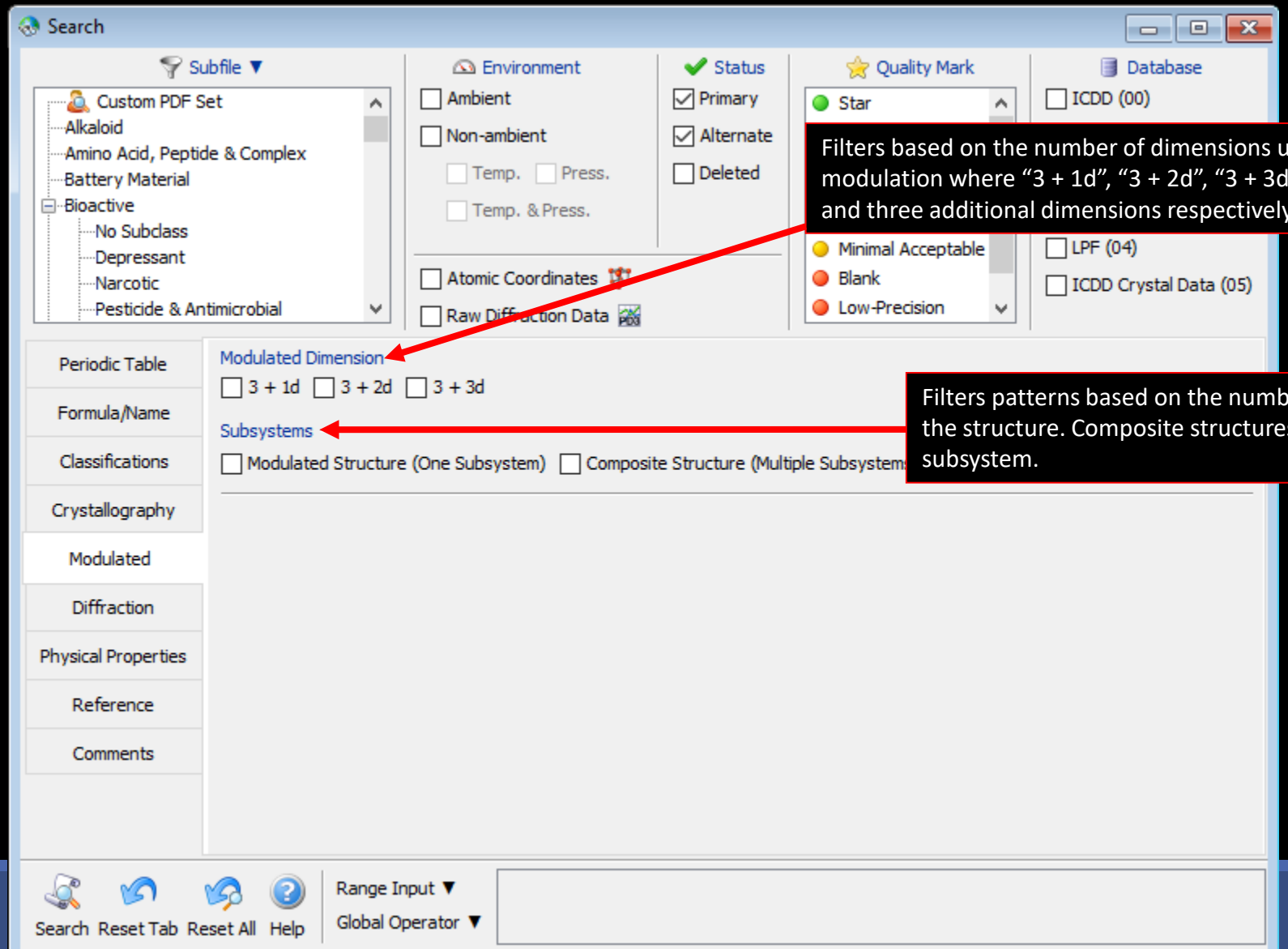
Supercell/Subcell

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.



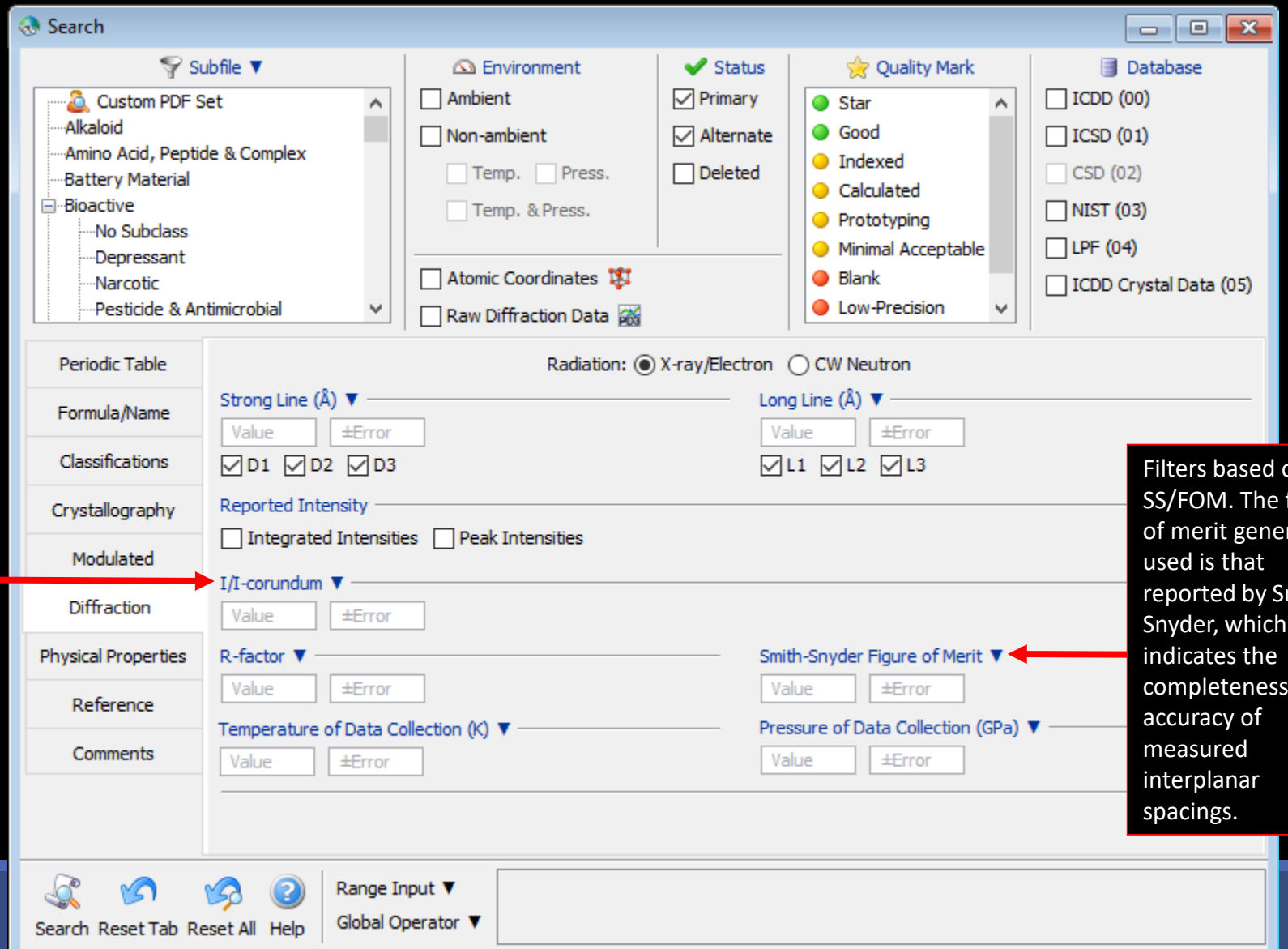
Search Window

Modulated



Search Window

Diffraction

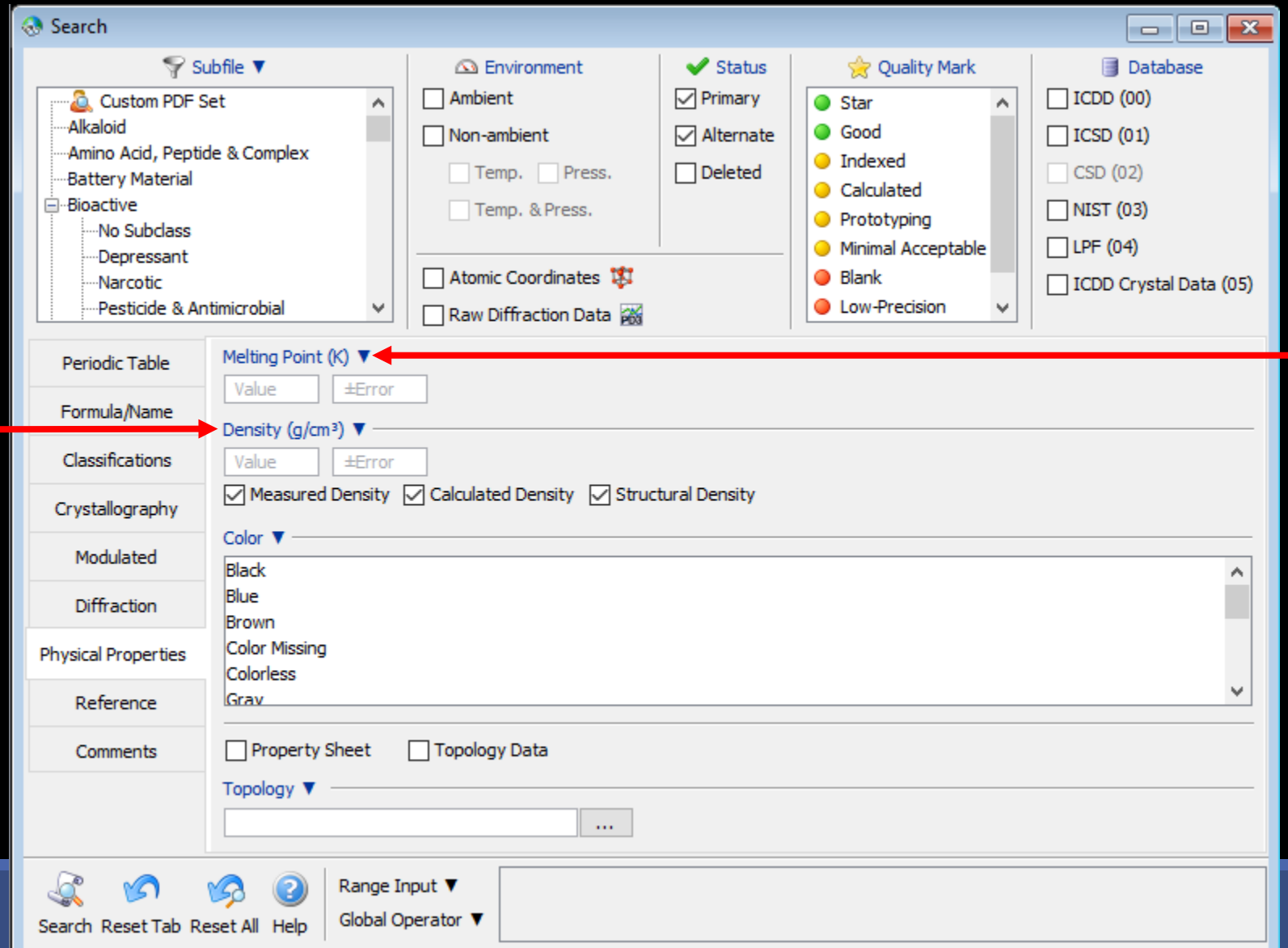


Filters based on the ratio of the intensity of the strongest line of the pattern to the intensity of the strongest line of corundum in a 50/50 weight mixture.

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

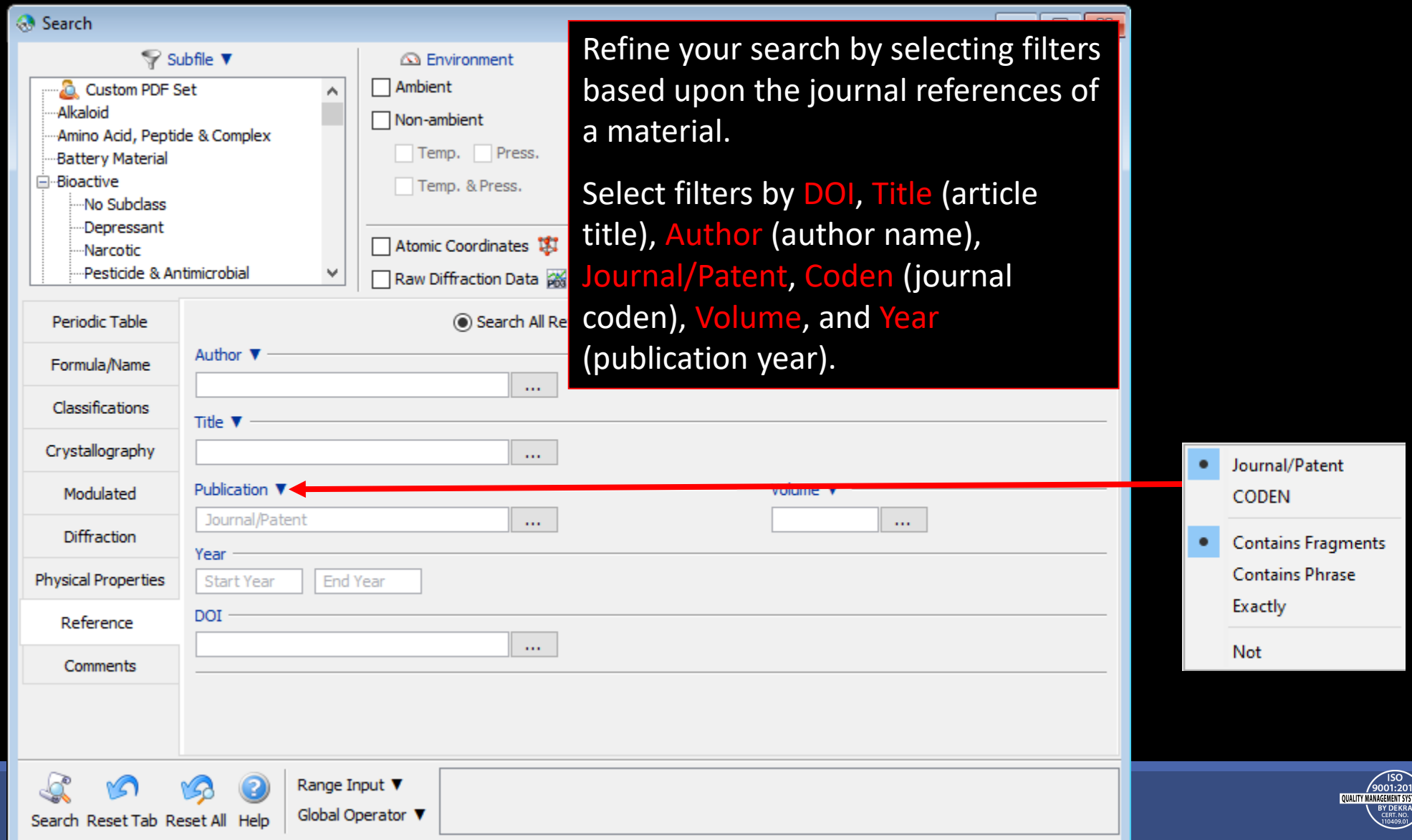


Filters based on the measured, calculated or structural density of the material.

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

Search Window

References

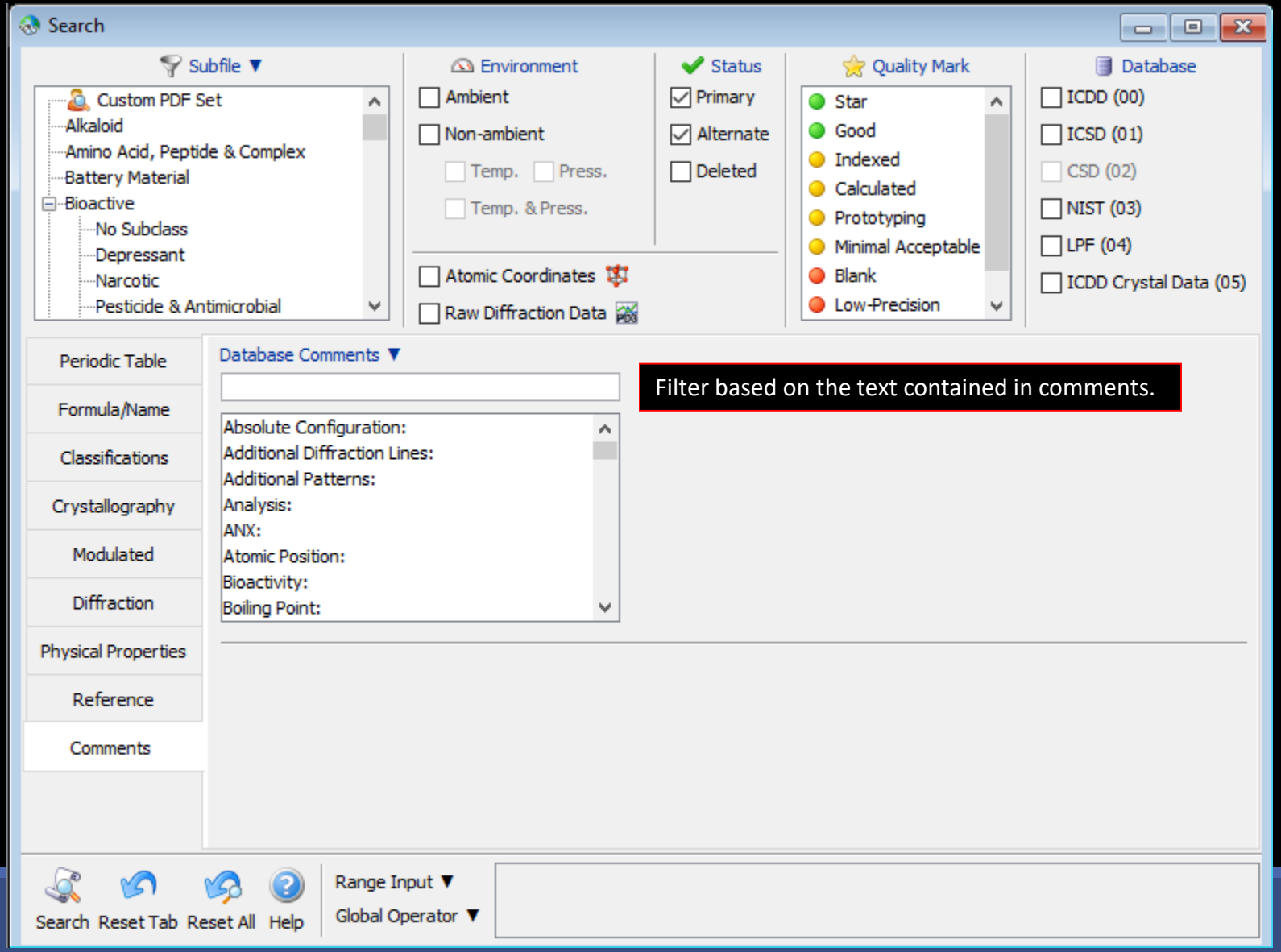


Refine your search by selecting filters based upon the journal references of a material.

Select filters by DOI, Title (article title), Author (author name), Journal/Patent, Coden (journal coden), Volume, and Year (publication year).

Search Window

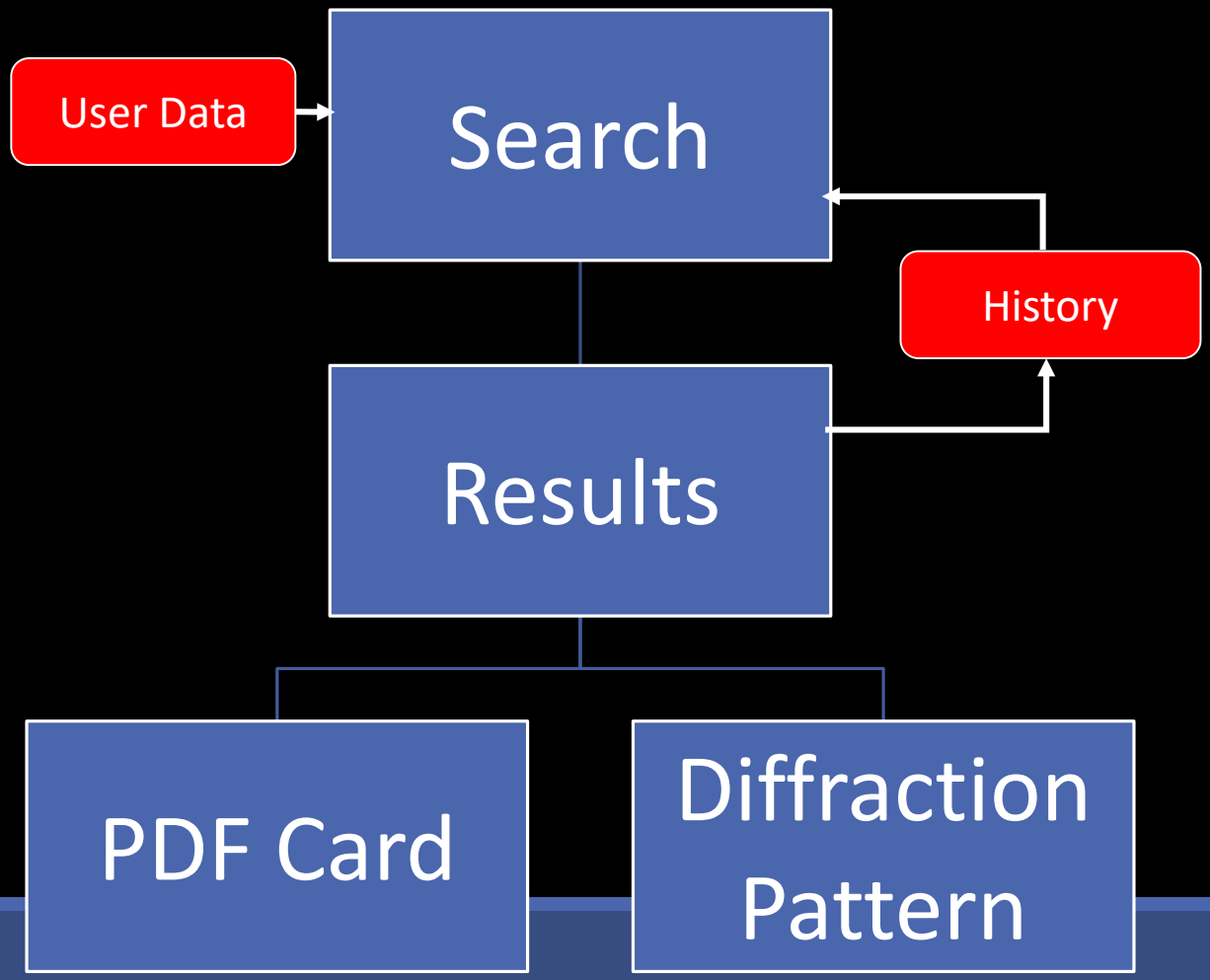
Comments



Data Mining Basics

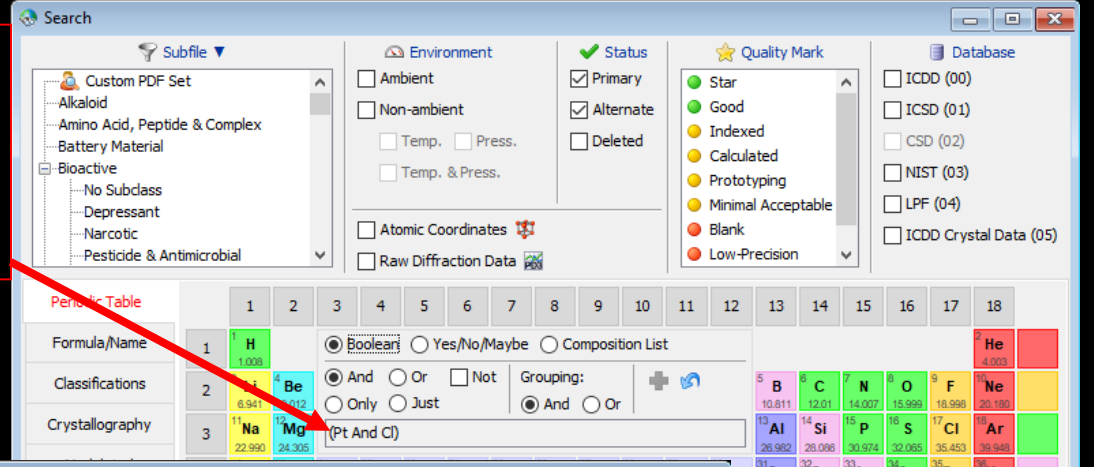
- Select your filter criteria
- Make use of logical Boolean operators, text and list boxes
- Search
- Review results
- Refine search with additional criteria

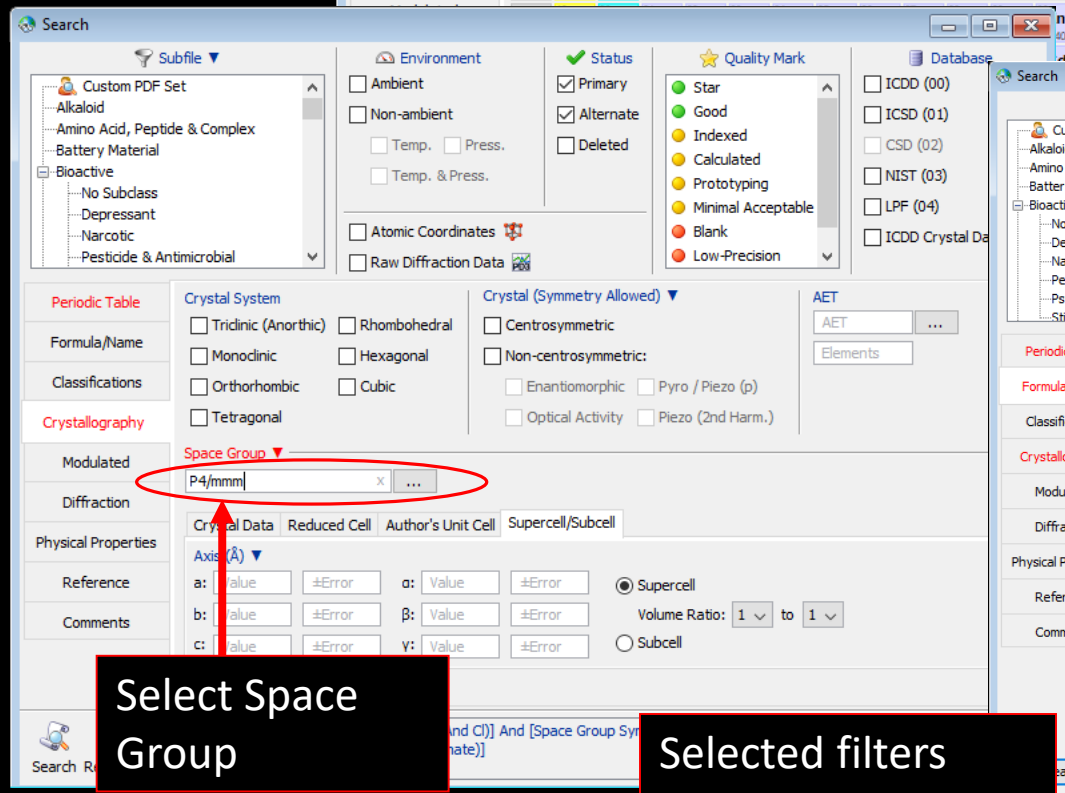
Note: Selected search criteria is highlighted in red to keep track of your selections.



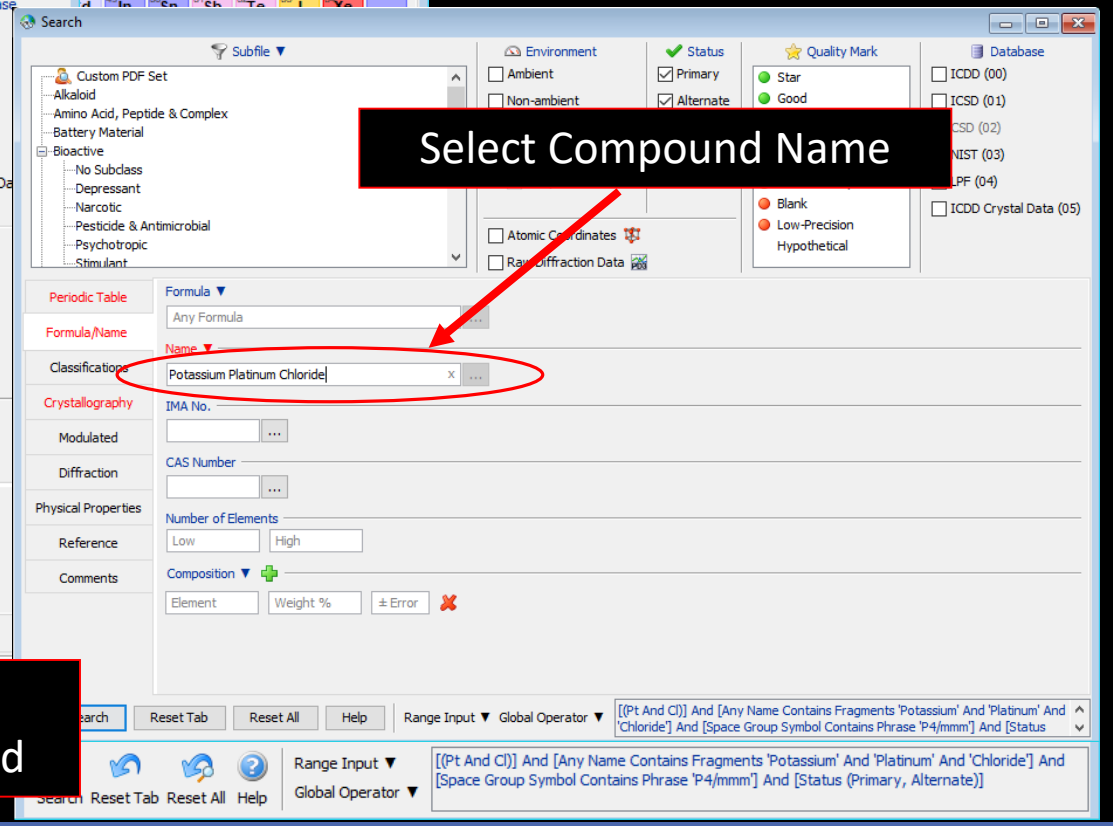
Search Example

Select Elements in Periodic Table





Select Space Group

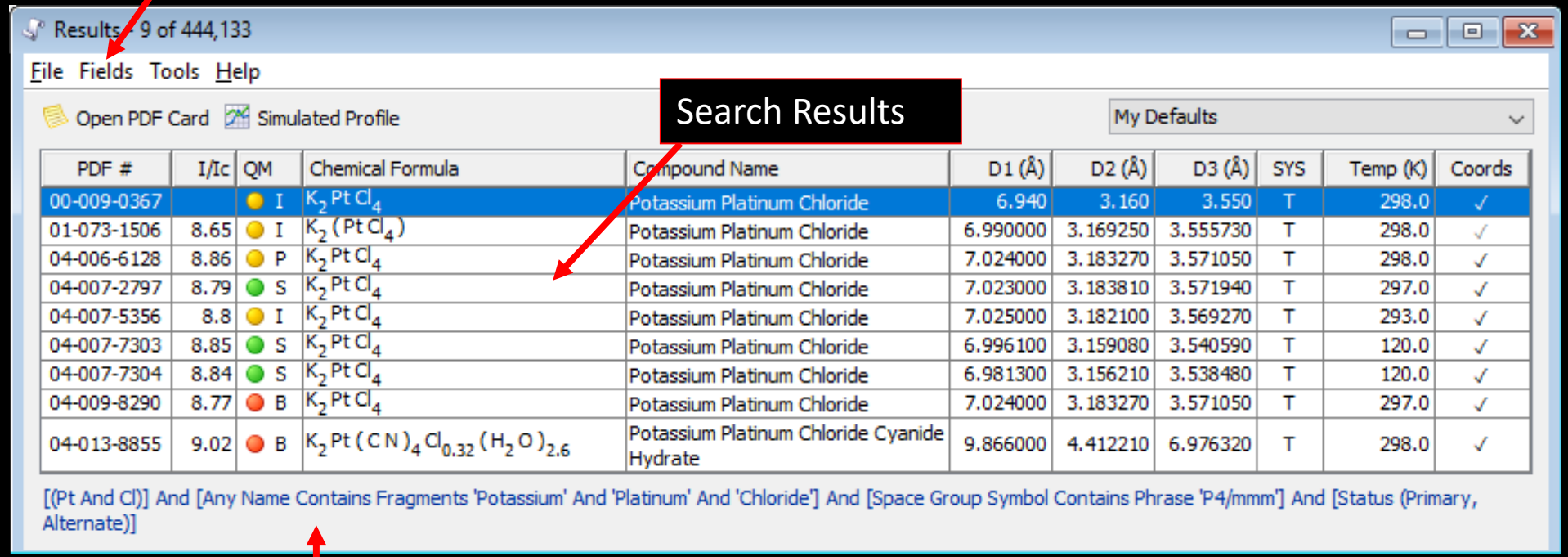


Select Compound Name

Selected filters highlighted in red

Search Results

Choose fields to be displayed in results



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

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

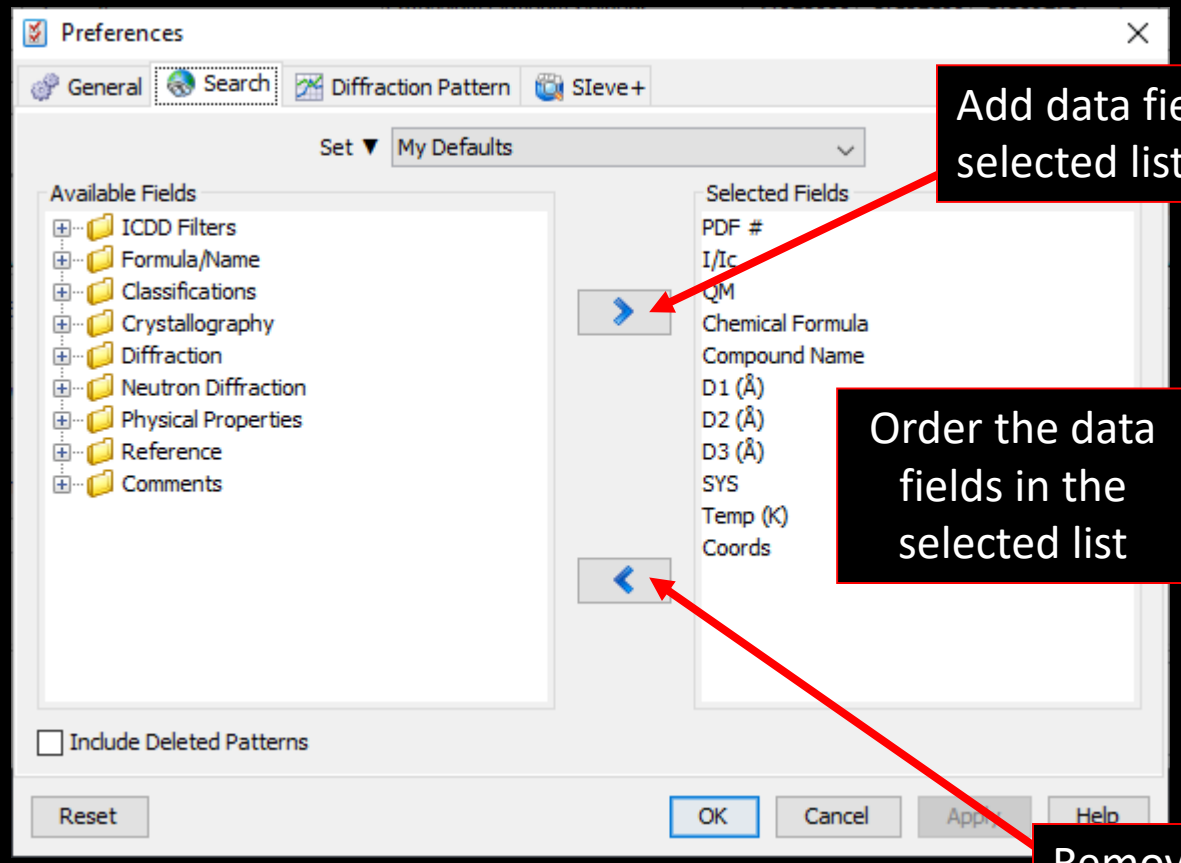
Search Filters

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

Preferences Module

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

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



Add data fields to selected list

Order the data fields in the selected list

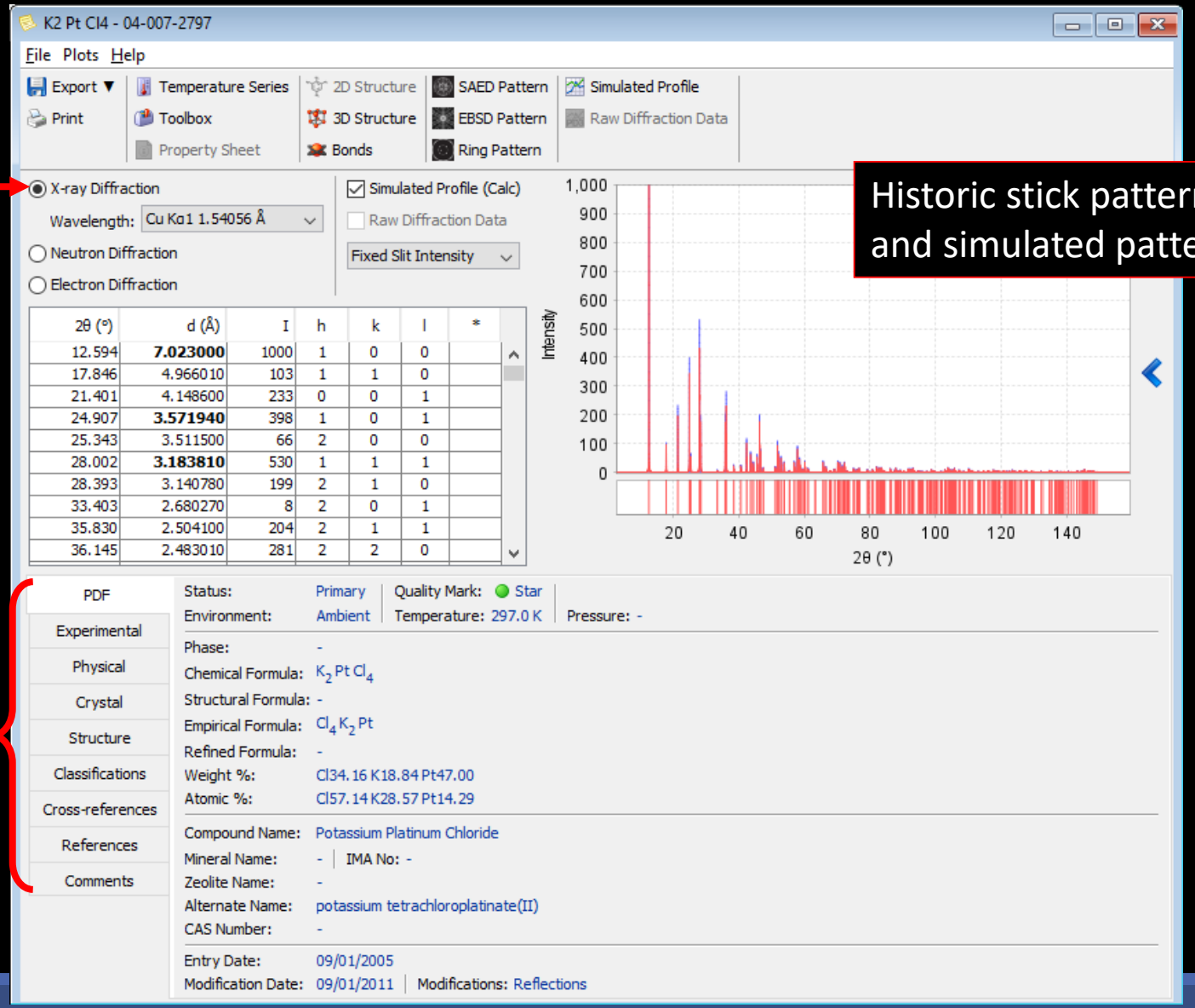
Remove data fields from the selected list

PDF Data Card

Choose equipment factors

Historic stick pattern and simulated pattern

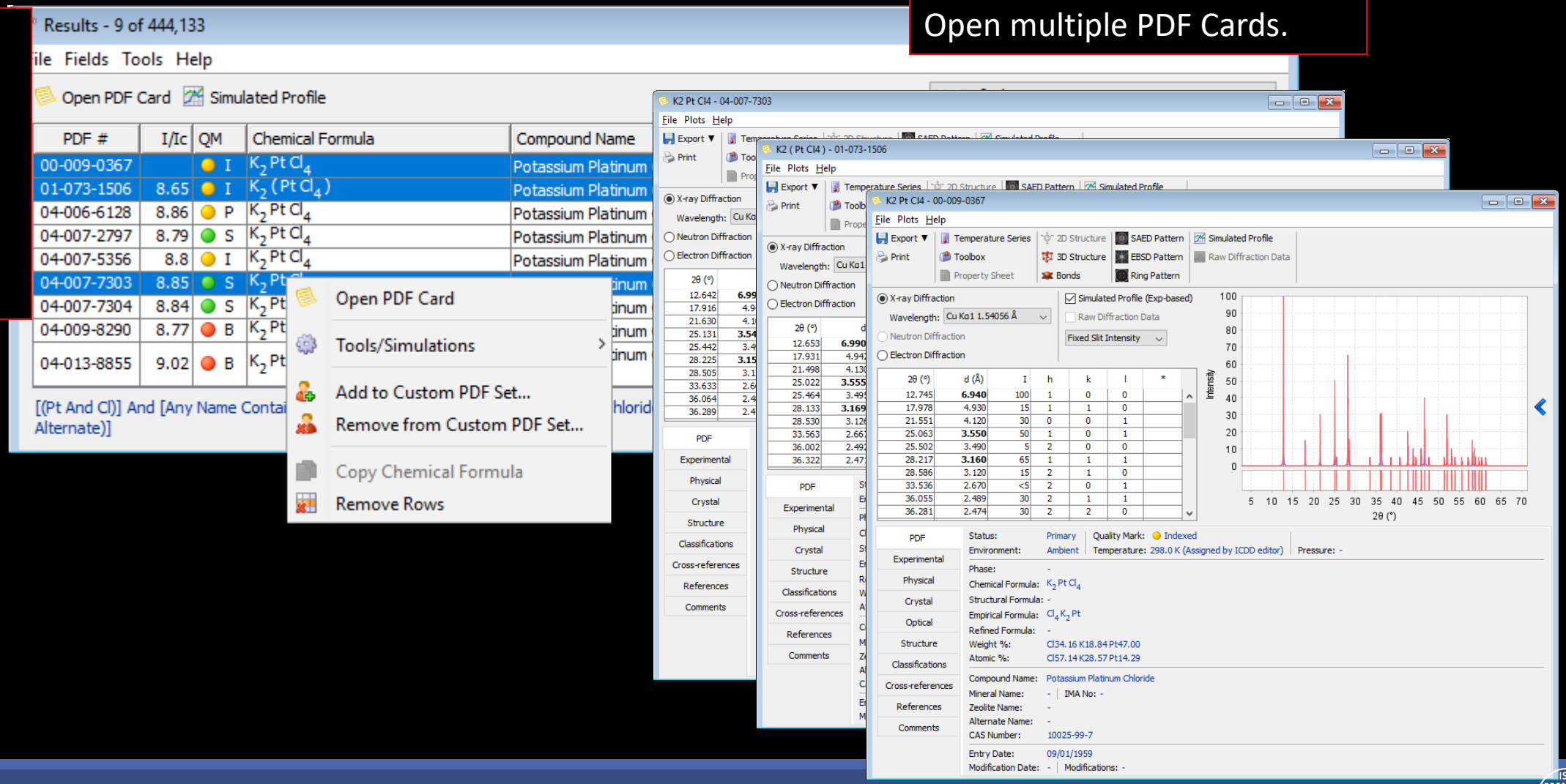
Tabular view of reported data



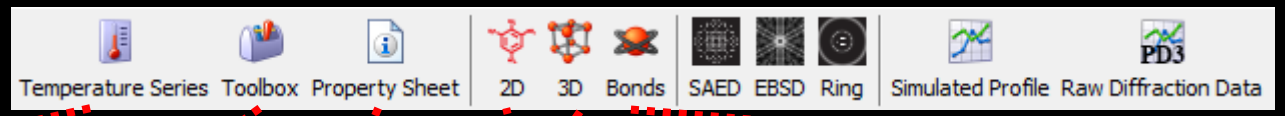
PDF Data Card

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

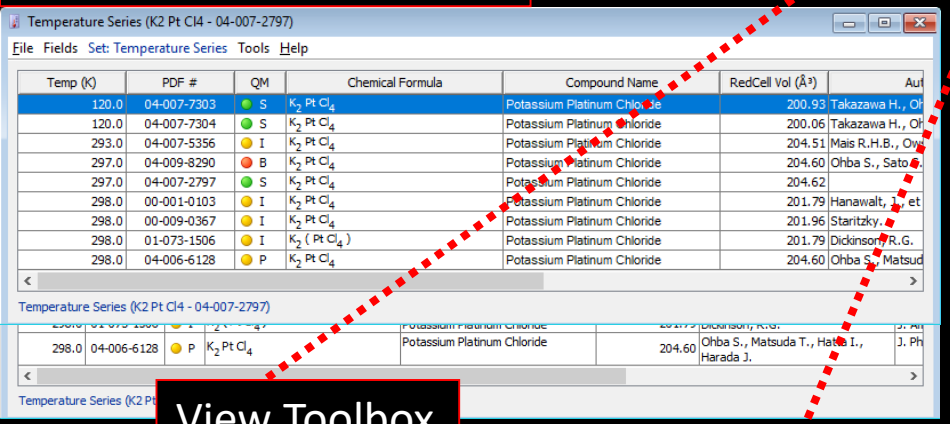
Open multiple PDF Cards.



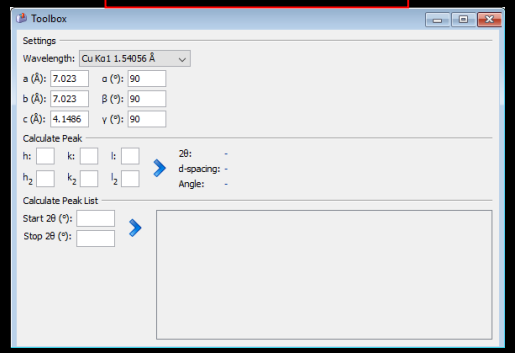
PDF Data Card Features



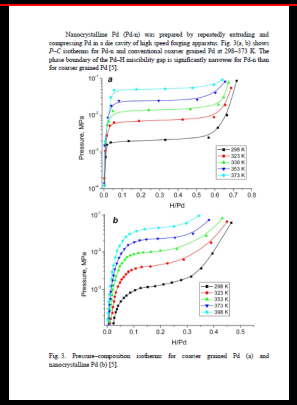
View Temperature Series



View Toolbox



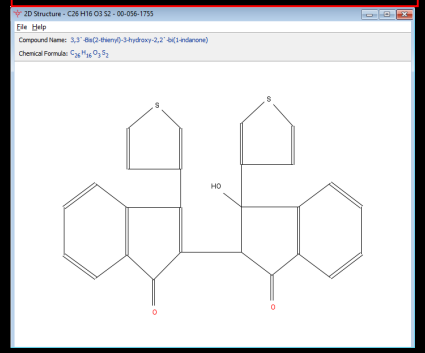
View Property Sheet



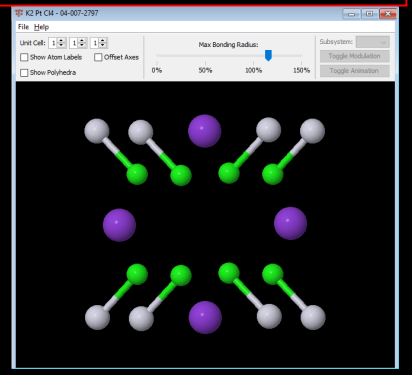
Nanocrystalline Pd (Pd-n) was prepared by repeatedly extruding and compressing Pd in a die cavity of high speed forging apparatus. Fig. 3(a, b) shows P–C isotherms for Pd-n and conventional coarser grained Pd at 296–373 K. The phase boundary of the Pd–H miscibility gap is significantly narrower for Pd-n than for coarser grained Pd [5].

Fig. 3. Pressure–composition isotherms for coarser grained Pd (a) and nanocrystalline Pd (b) [5].

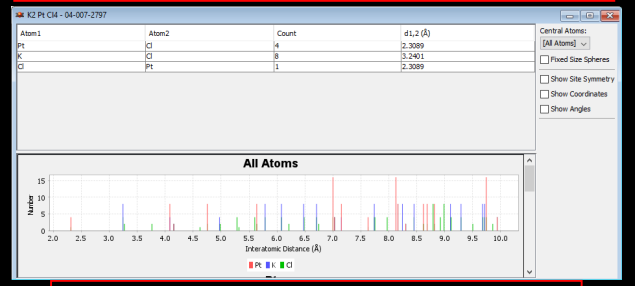
View 2D Structure



View 3D Structure

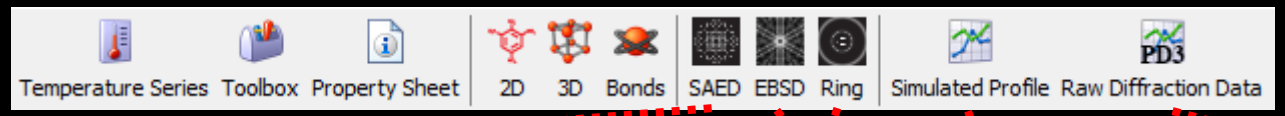


View Bond Distances/Angles

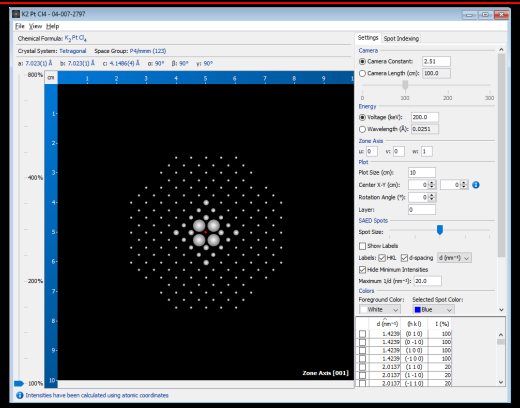


Note: The availability of each feature varies by PDF entry.

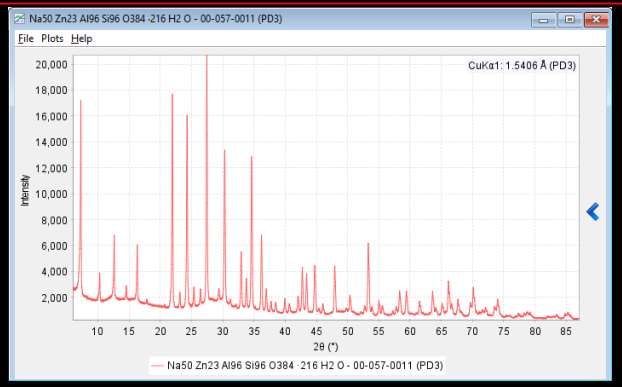
PDF Data Card Features



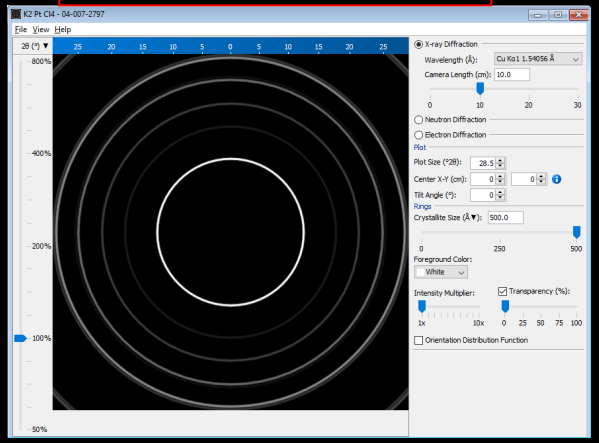
View Simulated Electron Spot Pattern



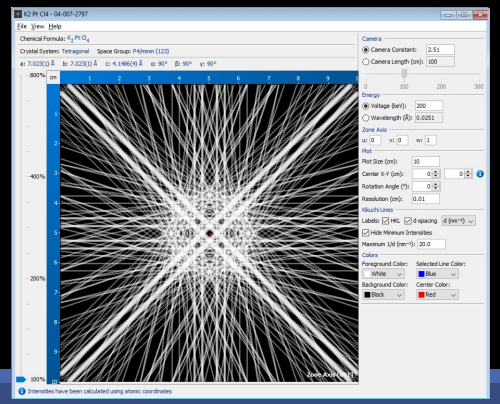
View Raw Diffraction Data (PD3)



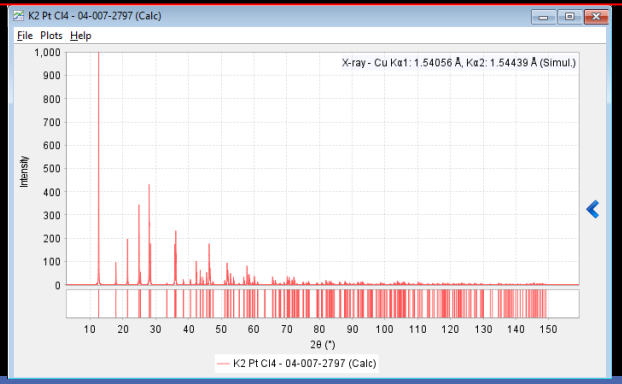
View Ring Pattern



View Electron Backscattering Pattern



View Simulated Diffraction Profile



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