

# The Subfile Search

In this tutorial, the following Topics are covered:

1. What is a Subfile?
2. How is a Subfile defined?
3. Learn more about a Subfile.
4. Why use a Subfile?
5. How to perform a Subfile search.

# What is a Subfile?

- The ICDD Subfile is a grouping of materials based on their chemistry or field of application.
- Considerable editorial effort is involved in defining a Subfile. This effort is on-going and subfile definitions are ever-evolving.

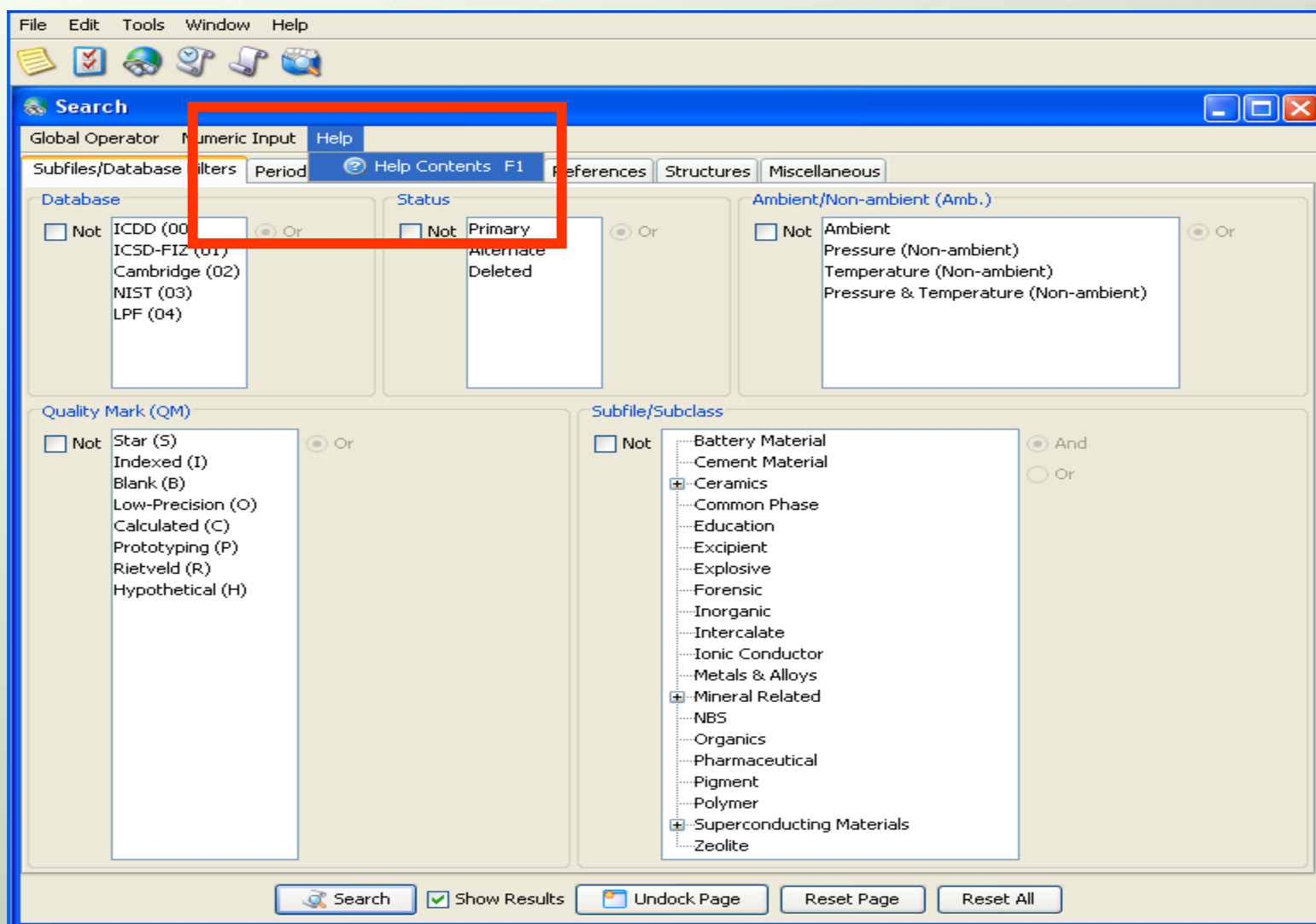
# How is a Subfile Defined?

- Subfiles may be defined in any of the following ways:
  - Chemical formula
    - Metals & Alloys, some Explosives
  - Physical property characteristics
    - Ionic conductors, Ferroelectrics
  - Structural and/or crystallographic features
    - Perovskites, Polymers, Zeolites
  - By the material's use
    - Bioceramics, Cement materials, Excipients

The Subfile Help Document:  
More information about a subfile  
may be found in the [Help Contents](#)

For more information about a specific Subfile, check the [Help Contents](#).

To open the Help document click on the word [Help](#) or press the [F1](#) key on your keyboard.



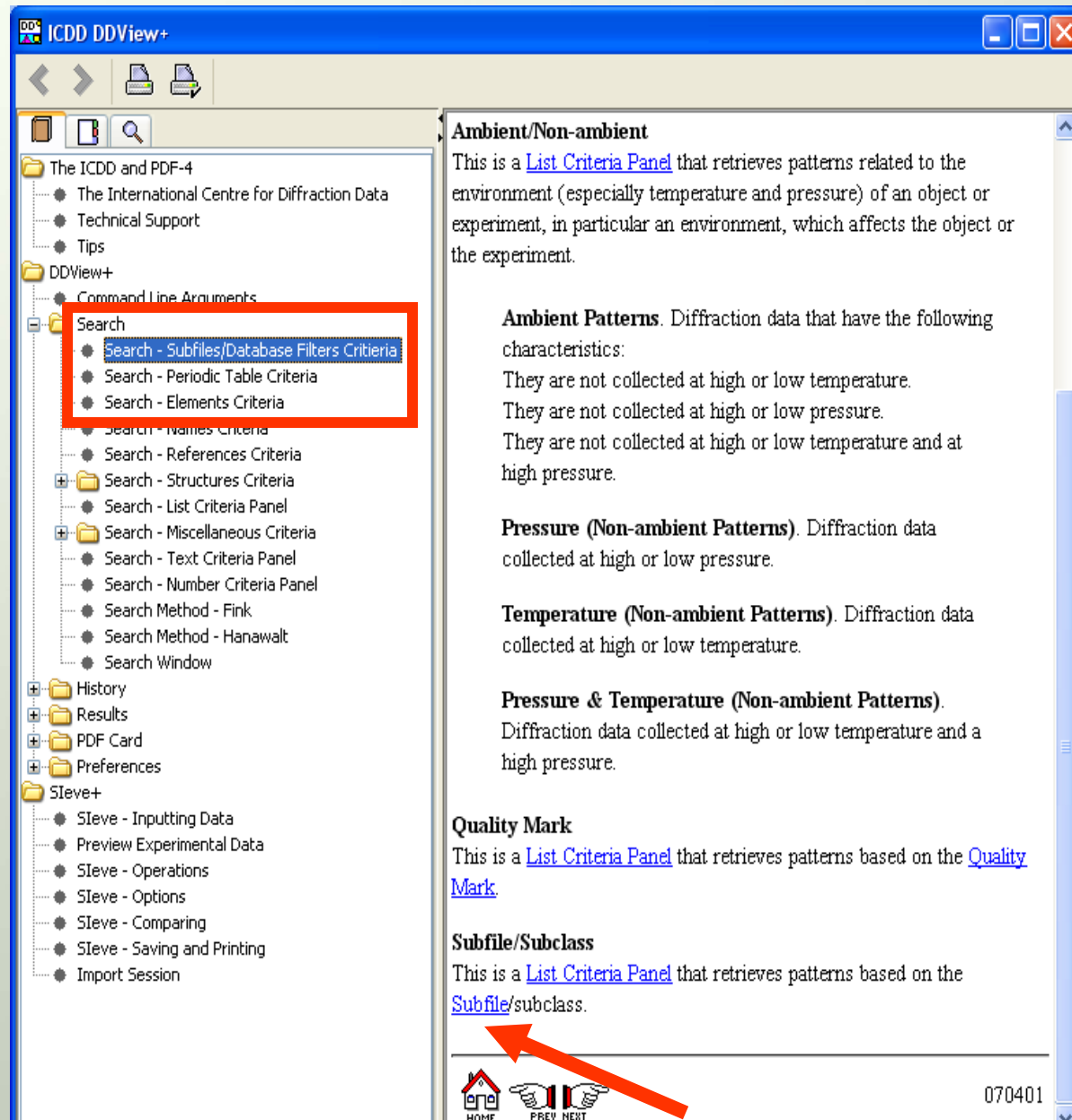
The screenshot shows the ICDD Search application window. The top menu bar includes File, Edit, Tools, Window, and Help. Below the menu is a toolbar with icons for search, help, and other functions. The main window has a blue header with the word "Search" and a search icon. Below the header is a navigation bar with tabs: Global Operator, Numeric Input, Help, Subfiles/Database filters, Period, Help Contents F1, References, Structures, and Miscellaneous. The "Help Contents F1" tab is selected and highlighted with a red box. The main content area is divided into several sections: Database (with checkboxes for Not, ICDD (00), ICSD-FIZ (01), Cambridge (02), NIST (03), LPF (04)), Status (with checkboxes for Not, Primary, Alternate, Deleted), Ambient/Non-ambient (Amb.) (with checkboxes for Not, Ambient, Pressure (Non-ambient), Temperature (Non-ambient), Pressure & Temperature (Non-ambient)), Quality Mark (QM) (with checkboxes for Not, Star (S), Indexed (I), Blank (B), Low-Precision (O), Calculated (C), Prototyping (P), Rietveld (R), Hypothetical (H)), and Subfile/Subclass (with checkboxes for Not, Battery Material, Cement Material, Ceramics, Common Phase, Education, Excipient, Explosive, Forensic, Inorganic, Intercalate, Ionic Conductor, Metals & Alloys, Mineral Related, NBS, Organics, Pharmaceutical, Pigment, Polymer, Superconducting Materials, Zeolite). At the bottom of the window are buttons for Search, Show Results, Undock Page, Reset Page, and Reset All.

# The Subfile Help document

Within the help Document, open the **Search** folder.

Then click on **Subfiles/ Database Filters Criteria**

Scroll to the Bottom of the subfile page, click on the **Subfile** link indicated to the right by the red arrow.



The screenshot shows the ICDD DDView+ application window. The left sidebar displays a tree view of the help document structure. The 'Search' folder is expanded, and the 'Search - Subfiles/Database Filters Criteria' item is highlighted with a red box. The main content area displays the help text for 'Subfile/Subclass', which includes a red arrow pointing to the 'Subfile/subclass' link at the bottom of the page. The text in the main area is as follows:

**Ambient/Non-ambient**  
This is a [List Criteria Panel](#) that retrieves patterns related to the environment (especially temperature and pressure) of an object or experiment, in particular an environment, which affects the object or the experiment.

**Ambient Patterns.** Diffraction data that have the following characteristics:  
They are not collected at high or low temperature.  
They are not collected at high or low pressure.  
They are not collected at high or low temperature and at high pressure.

**Pressure (Non-ambient Patterns).** Diffraction data collected at high or low pressure.

**Temperature (Non-ambient Patterns).** Diffraction data collected at high or low temperature.

**Pressure & Temperature (Non-ambient Patterns).** Diffraction data collected at high or low temperature and a high pressure.

**Quality Mark**  
This is a [List Criteria Panel](#) that retrieves patterns based on the [Quality Mark](#).

**Subfile/Subclass**  
This is a [List Criteria Panel](#) that retrieves patterns based on the [Subfile/subclass](#).

At the bottom of the window, there are navigation icons: a home icon, a hand icon, and a 'PREV NEXT' button. The number '070401' is displayed in the bottom right corner.

# Information about Subfiles Contained in the Help Document

- Subfile Consultants:
  - Names of editors involved in creating the subfile definitions.
- Key References:
  - References used in creating the definition
- Subfile History:
  - A brief history of the origin of the subfile.
- Subfile Definition
- May contain examples of what is and what is NOT included in the subfile.

# Why Use a Subfile?

- The Powder Diffraction File (PDF-4+) contains over 285,000 materials.
- Subfiles speed your search by including only those materials you are interested in.

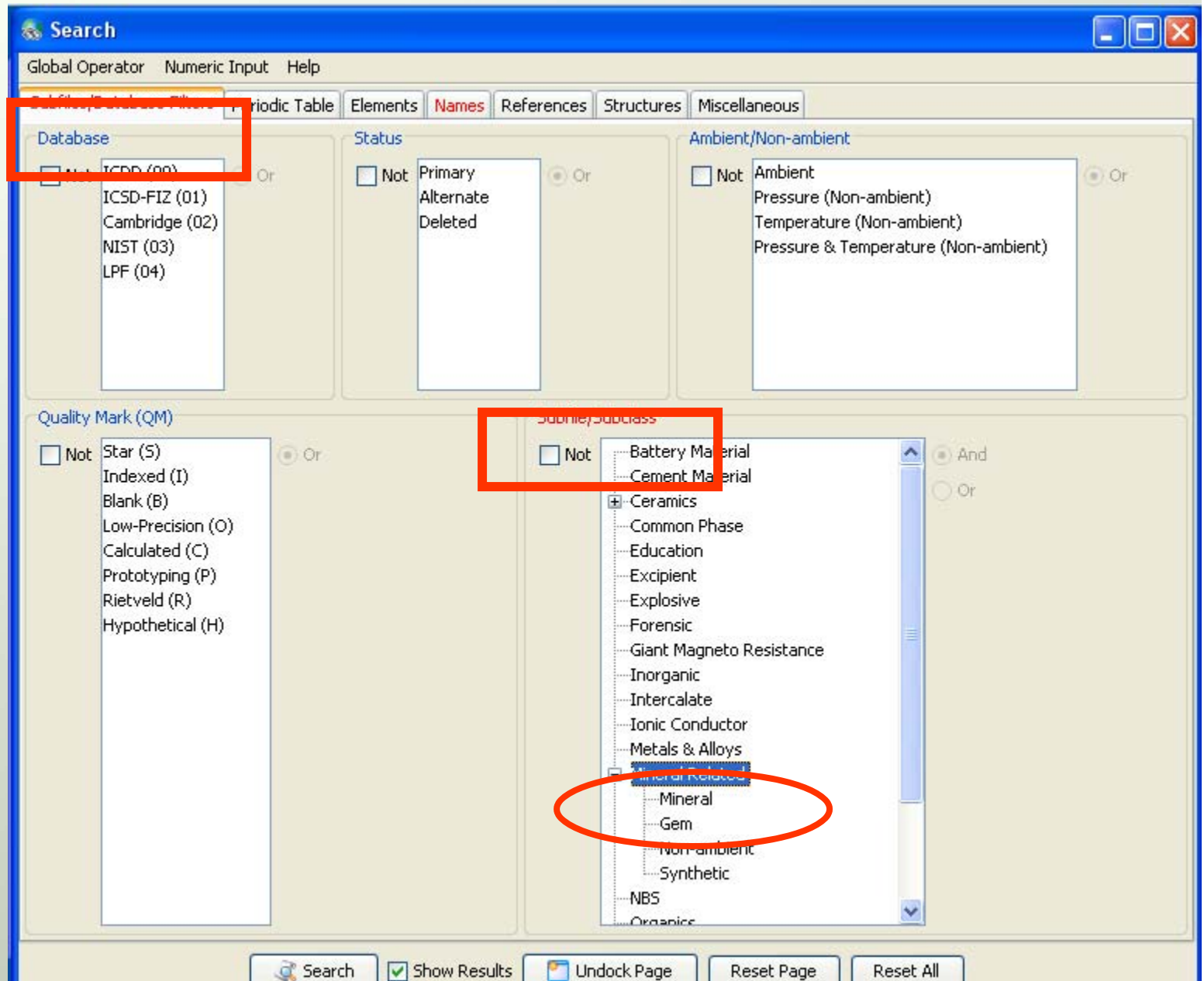
# How to perform a Subfile Search

This is the **SubFiles/ Database Filters** pane.

The **Subfile/ Subclass** panel is highlighted

The Subfile: **Mineral Related** has been chosen.

Notice the Subclasses under the Mineral Related Subfile.



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

- Database:** ICDD (00) is selected. Other options include ICSD-FIZ (01), Cambridge (02), NIST (03), and LPF (04).
- Status:** Primary, Alternate, and Deleted are listed.
- Ambient/Non-ambient:** Ambient, Pressure (Non-ambient), Temperature (Non-ambient), and Pressure & Temperature (Non-ambient) are listed.
- Quality Mark (QM):** Star (S), Indexed (I), Blank (B), Low-Precision (O), Calculated (C), Prototyping (P), Rietveld (R), and Hypothetical (H) are listed.
- Subfile/Subclass:** A list of subfiles is shown, with 'Mineral Related' selected and highlighted. Under 'Mineral Related', 'Mineral' and 'Gem' are also highlighted.

Buttons at the bottom include: Search, Show Results, Undock Page, Reset Page, and Reset All.



Searching for **Battery materials** is a general search and will return all such materials.

However, if we are only interested in batteries containing Lithium, we may further narrow our search using the **Periodic Table** pane.

To reach the **Periodic Table** pane, click on the tab indicated by the red arrow and labeled **Periodic Table**

# Let's look at Battery Materials

The screenshot shows the 'Global Operator' search interface. At the top, there are menu items: 'Global Operator', 'Numeric Input', and 'Help'. Below the menu is a row of tabs: 'Subfiles/Database Filters', 'Periodic Table', 'Elements', 'Names', 'References', 'Structures', and 'Miscellaneous'. A red arrow points to the 'Periodic Table' tab. The main area is divided into several filter sections:

- Database:** Includes checkboxes for 'Not' and 'Or' with a list of databases: ICDD (00), ICSD-FIZ (01), Cambridge (02), NIST (03), and LPF (04).
- Status:** Includes checkboxes for 'Not' and 'Or' with a list of statuses: Primary, Alternate, and Deleted.
- Ambient/Non-ambient:** Includes checkboxes for 'Not' and 'Or' with a list of conditions: Ambient, Pressure (Non-ambient), Temperature (Non-ambient), and Pressure & Temperature (Non-ambient).
- Quality Mark (QM):** Includes checkboxes for 'Not' and 'Or' with a list of quality marks: Star (S), Indexed (I), Blank (B), Low-Precision (O), Calculated (C), Prototyping (P), Rietveld (R), and Hypothetical (H).
- Subfile/Subclass:** Includes checkboxes for 'Not', 'And', and 'Or' with a tree view of material classes. 'Battery Material' is highlighted in blue. Other classes include Cement Material, Ceramics, Common Phase, Education, Excipient, Explosive, Forensic, Giant Magneto Resistance, Inorganic, Intercalate, Ionic Conductor, Metals & Alloys, Mineral Related (with sub-items Mineral, Gem, Non-ambient, Synthetic), NBS, and Organic.

At the bottom of the interface, there are five buttons: 'Search', 'Show Results' (with a checked checkbox), 'Undock Page', 'Reset Page', and 'Reset All'.

Search

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements Names References Structures Miscellaneous

IA IIA IIIB IVB VB VIB VIIB VIIIB IB IIB IIIA IVA VA VIA VIIA VIIIA

Period 1 1 H 1.008 2 He 4.003

Period 2 3 Li 6.941 4 Be 9.012 5 B 10.811 6 C 12.011 7 N 14.007 8 O 15.999 9 F 18.998 10 Ne 20.180

Period 3 11 Na 22.990 12 Mg 24.305 13 Al 26.982 14 Si 28.086 15 P 30.974 16 S 32.064 17 Cl 35.453 18 Ar 39.948

Period 4 19 K 39.098 20 Ca 40.08 21 Sc 44.956 22 Ti 47.88 23 V 50.942 24 Cr 51.996 25 Mn 54.938 26 Fe 55.847 27 Co 58.993 28 Ni 58.69 29 Cu 63.546 30 Zn 65.38 31 Ga 69.72 32 Ge 72.61 33 As 74.922 34 Se 78.96 35 Br 79.904 36 Kr 83.80

Period 5 37 Rb 85.47 38 Sr 87.62 39 Y 88.906 40 Zr 91.22 41 Nb 92.906 42 Mo 95.94 43 Tc 98 44 Ru 101.07 45 Rh 102.91 46 Pd 106.4 47 Ag 107.87 48 Cd 112.41 49 In 114.82 50 Sn 118.69 51 Sb 121.75 52 Te 127.60 53 I 126.90 54 Xe 126.90

Period 6 55 Cs 132.91 56 Ba 137.33 72 Hf 178.49 73 Ta 180.95 74 W 183.85 75 Re 186.21 76 Os 190.2 77 Ir 192.2 78 Pt 195.08 79 Au 196.97 80 Hg 200.59 81 Tl 204.38 82 Pb 207.19 83 Bi 208.98 84 Po 209 85 At 210 86 Rn 222

Period 7 87 Fr 223 88 Ra 226.03

LN: 57 La 138.91 58 Ce 132.91 59 Pr 140.91 60 Nd 144.24 61 Pm 145 62 Sm 150.36 63 Eu 151.97 64 Gd 157.25 65 Tb 158.93 66 Dy 162.5 67 Ho 164.93 68 Er 167.26 69 Tm 168.93 70 Yb 173.04 71 Lu 174.97

AC: 89 Ac 227.03 90 Th 232.04 91 Pa 231.04 92 U 238.03 93 Np 237.05 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 260

Inner Operators:  Not  And  Or

Outer Operators:  And  Or

+ Add

Undo

Search Show Results Undock Page Reset Page Reset All

Search PDF Card - 01-070-1620

On the Periodic Table pane, click on Li.

Then click on the Add button indicated by the red arrow.

This search is more specific and returns a subset of all the battery materials.

# Conclusion

- Subfiles are a convenient way to classify the enormous amount of data in the PDF.
- Classifications are based on the chemistry, structure or application of the material.
- If the user knows something about the chemistry of the compound to be analyzed, the search can be greatly facilitated by the use of the appropriate subfile.



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



International Centre for Diffraction Data

12 Campus Boulevard

Newtown Square, PA 19073

Phone: 610.325.9814

Fax: 610.325.9823