

Sort, Order and Graph Data

Sort and Order

- What?
 - Sorting is the ability to order the PDF data retrieved from the search results.
- Why?
 - To organize the data.
 - To find relevant data faster and easier.
- How?
 - Use the Results table.

Results Table

- The Results table can be sorted on any display field.
- Depending on the display field sorted, there are different types of sorting available:
 - Alphabetical Sort
 - Numerical Sort
 - Special Order Sort
 - Alphabetical Formula Index Sort

Alphabetical Sort

- The Alphabetical Sort will sort a text-based column alphabetically from A - Z.
- This can be performed by:
 - Left-clicking a text-based sort column (e.g., Compound Name).
 - Or middle-clicking a *Special Order* Sort column (e.g., QM).
 - Or right-clicking a text-based sort column and selecting *Sort Alphabetically*.
- Sorting on a *Special Order* Sort column will override the *Special Order* Sort.
- Sorting on a column twice will perform a descending sort from Z – A.

Results (148 of 316,291)

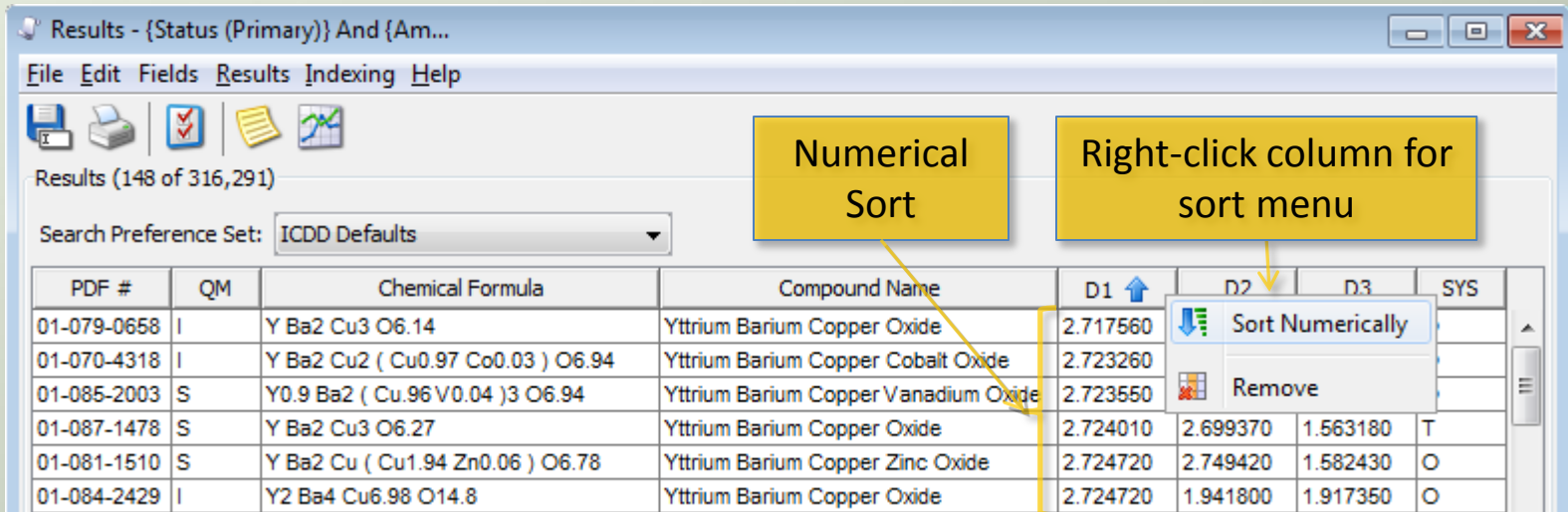
Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D3	SYS
01-081-1200	S	D0.61 Y2 Ba Cu O5	Deuterium Yttrium Barium Copper	2.827500	O
01-081-1201	B	D1.31 Y2 Ba Cu O5	Deuterium Yttrium Barium Copper	2.934430	O
01-078-2242	S	La.75 Y.75 Ba1.5 Cu3 O7	Lanthanum Yttrium Barium Copper Oxide	1.937300	T
01-078-2243	S	(La.25 Y.75) (Ba1.5 La.5) Cu3 O6.7...	Lanthanum Yttrium Barium Copper Oxide	1.934650	T
01-074-7571	B	Pb Y Ba2 Cu3 O7 F2	Lead Yttrium Barium Copper Oxide Flu...	1.933300	T
01-087-0230	S	(Nd0.6 Y0.4) Ba2 Cu2.95 O6.76	Neodymium Yttrium Barium Copper Oxi...	1.584430	O

Sorted by Compound Name

Numerical Sort

- The *Numerical Sort* will sort a numerical column from 0 – 999...
- This can be performed by:
 - Left-clicking a numerical sort column (e.g., D1).
 - Or right-clicking a numerical sort column and selecting *Sort Numerically*.
- Sorting on a column twice will perform a descending sort from 999... – 0.



Results (148 of 316,291)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D1 ↑	D2 ↓	D3	SYS
01-079-0658	I	Y Ba2 Cu3 O6.14	Yttrium Barium Copper Oxide	2.717560			
01-070-4318	I	Y Ba2 Cu2 (Cu0.97 Co0.03) O6.94	Yttrium Barium Copper Cobalt Oxide	2.723260			
01-085-2003	S	Y0.9 Ba2 (Cu.96 V0.04)3 O6.94	Yttrium Barium Copper Vanadium Oxide	2.723550			
01-087-1478	S	Y Ba2 Cu3 O6.27	Yttrium Barium Copper Oxide	2.724010	2.699370	1.563180	T
01-081-1510	S	Y Ba2 Cu (Cu1.94 Zn0.06) O6.78	Yttrium Barium Copper Zinc Oxide	2.724720	2.749420	1.582430	O
01-084-2429	I	Y2 Ba4 Cu6.98 O14.8	Yttrium Barium Copper Oxide	2.724720	1.941800	1.917350	O

Sorted by D1 (Strongest line)

Special Order Sort

- The *Special Order Sort* will sort a text-based column using an ordering specific to that column. The *Special Order Sort* columns are:
- PDF # (Powder Diffraction File Number)
 - This first orders the PDF #'s by database code: 00 (ICDD), 04 (LPF), 03 (NIST), 02 (CSD), 01 (ICSD).
 - This then orders the PDF #'s by descending set and card number (xx-###-####).
- QM (Quality Mark)
 - Ascending: S (Star), I (Indexed), B (Blank), O (Low-Precision), C (Calculated), P (Prototyping), R (Rietveld), H (Hypothetical)
 - Descending: C (Calculated), P (Prototyping), R (Rietveld), H (Hypothetical), S (Star), I (Indexed), B (Blank), O (Low-Precision)

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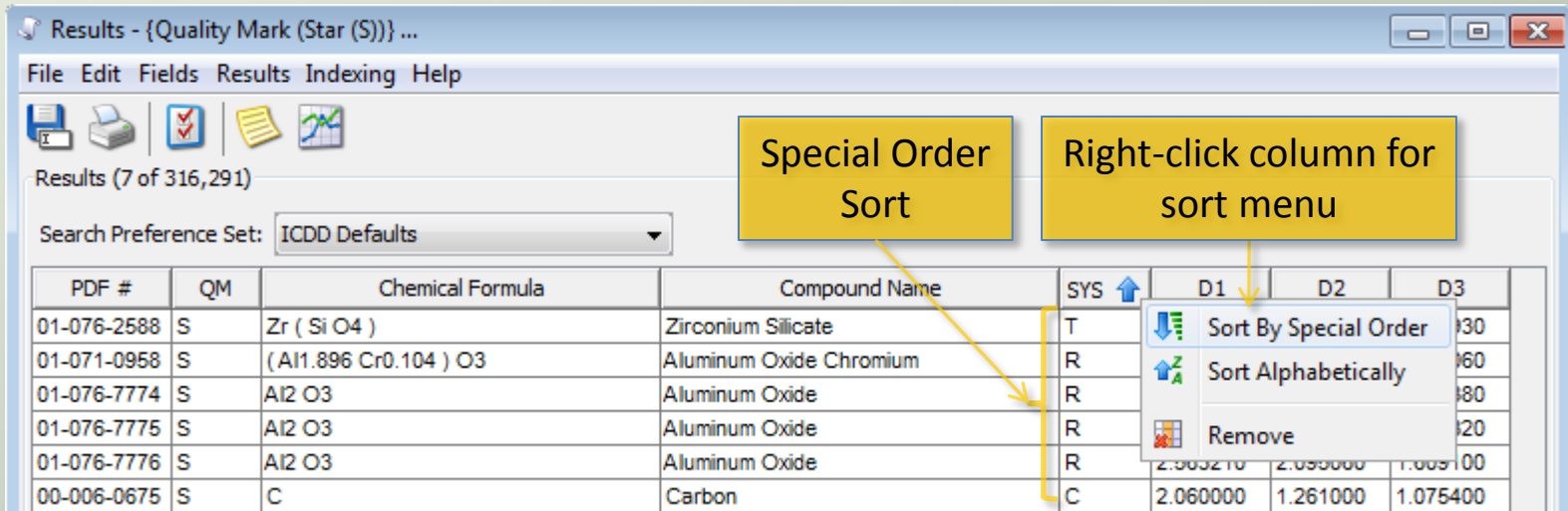
Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
01-081-1511	S	YBaCuZnO	Yttrium Barium Copper Zinc Oxide	2.728180	2.751440	1.582570	O
01-079-1227	S	YBaCuZnO	Yttrium Barium Copper Zinc Oxide	2.728630	2.751930	1.584460	O
01-081-1509	S	YBaCuZnO	Yttrium Barium Copper Zinc Oxide	2.729760	2.753540	1.584090	O
01-082-0187	I	YBaCuZnO	Thallium Yttrium Barium Copper Oxide	2.829490	2.733670	3.284700	T
01-079-1368	I	YBaCuZnO	Yttrium Barium Copper Aluminum Oxide	2.748590	2.738620	1.583060	T
01-070-4318	I	YBa ₂ Cu ₂ (Cu _{0.97} Co _{0.03})O _{6.94}	Yttrium Barium Copper Cobalt Oxide	2.723260	2.745850	1.580820	O

Sorted by QM (Quality Mark) showing S (Star) patterns first, as they are of the highest quality.

Special Order Sort

- **SYS (Crystal System)**
 - Ascending: A (Anorthic), M (Monoclinic), O (Orthorhombic), T (Tetragonal), H (Hexagonal), R (Rhombohedral), C (Cubic), X (Unassigned)
 - Descending: C (Cubic), R (Rhombohedral), H (Hexagonal), T (Tetragonal), O (Orthorhombic), M (Monoclinic), A (Anorthic), X (Unassigned)
- **Pearson (Pearson Symbol Code)**
 - This first orders by the Crystal Symmetry: a, m, o, t, h, c, ?
 - Secondly, this orders by the Lattice Centering: P, R, C, I, F, ?
 - Thirdly, this orders by the Atomic Count ascending.
- **Status**
 - Ascending: P (Primary), A (Alternate), D (Deleted)
 - Descending: D (Deleted), A (Alternate), P (Primary)



Results - {Quality Mark (Star (S))} ...

File Edit Fields Results Indexing Help

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Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	SYS ↑	D1	D2	D3
01-076-2588	S	Zr (Si O4)	Zirconium Silicate	T			130
01-071-0958	S	(Al1.896 Cr0.104) O3	Aluminum Oxide Chromium	R			160
01-076-7774	S	Al2 O3	Aluminum Oxide	R			180
01-076-7775	S	Al2 O3	Aluminum Oxide	R			120
01-076-7776	S	Al2 O3	Aluminum Oxide	R	2.365210	2.099000	1.009100
00-006-0675	S	C	Carbon	C	2.060000	1.261000	1.075400

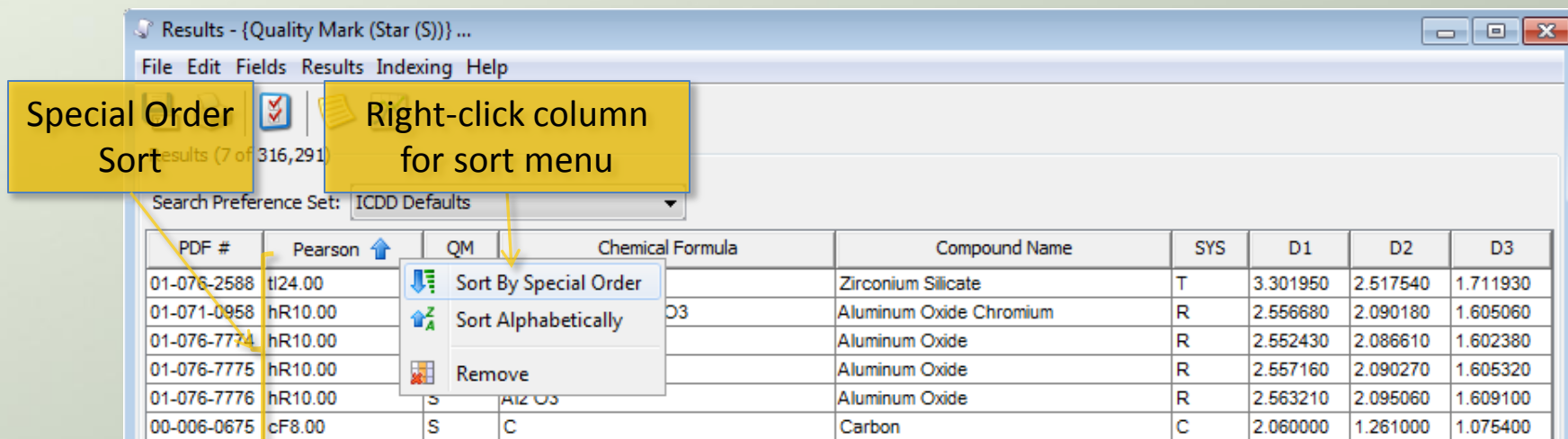
Context Menu Options:

- Sort By Special Order
- Sort Alphabetically
- Remove

Sorted by SYS (Crystal System)

Special Order Sort

- This can be performed by:
 - Left-clicking a *Special Order* sort column.
 - Or right-clicking a *Special Order* sort column and selecting *Sort by Special Order*.
- Sorting on a column twice will perform a descending sort.



Results - {Quality Mark (Star (S))} ...

File Edit Fields Results Indexing Help

Search Preference Set: ICDD Defaults

Special Order Sort

Right-click column for sort menu

PDF #	Pearson	Q#M	Chemical Formula	Compound Name	SYS	D1	D2	D3
01-076-2588	tI24.00			Zirconium Silicate	T	3.301950	2.517540	1.711930
01-071-0958	hR10.00		O3	Aluminum Oxide Chromium	R	2.556680	2.090180	1.605060
01-076-7774	hR10.00			Aluminum Oxide	R	2.552430	2.086610	1.602380
01-076-7775	hR10.00			Aluminum Oxide	R	2.557160	2.090270	1.605320
01-076-7776	hR10.00		Al2O3	Aluminum Oxide	R	2.563210	2.095060	1.609100
00-006-0675	cF8.00	S	C	Carbon	C	2.060000	1.261000	1.075400

Sort By Special Order

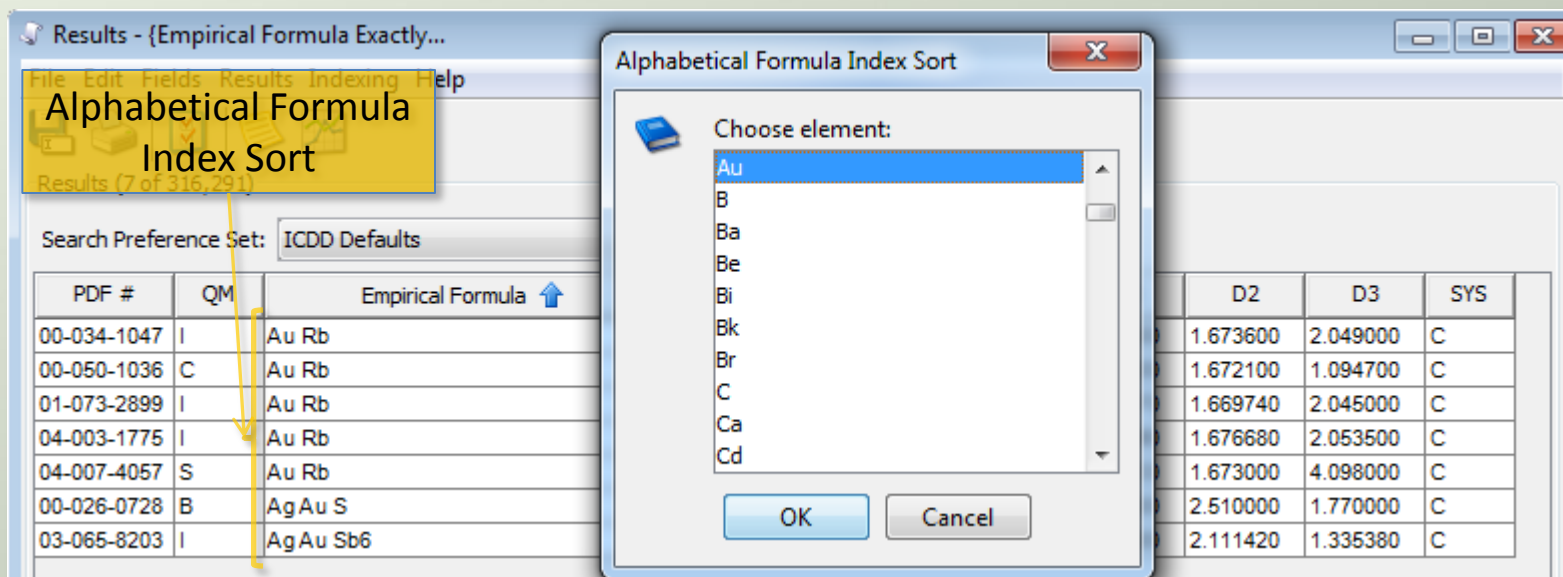
Sort Alphabetically

Remove

Sorted by Pearson Symbol Code

Alphabetical Formula Index Sort

- The *Alphabetical Formula Index Sort* will sort the Empirical Formula column based on a specific sort element.
- Formulae are sorted by elements alphabetically starting with the sort element.
- Example 1: **Al**, **Al S**, **Al Si** - sorted on **Al**
 - This example shows a basic alphabetical sort.
- Example 2: **Au Rb**, **Ag Au S**, **Ag Au Sb₆** - sorted on **Au**
 - Since sorting starts with the sorting element first, “Ag Au Sb₆” comes last because Rb comes before S and Sb.



Results - {Empirical Formula Exactly...}

File Edit Fields Results Indexing Help

Alphabetical Formula Index Sort

Search Preference Set: ICDD Defaults

PDF #	QM	Empirical Formula ↑
00-034-1047	I	Au Rb
00-050-1036	C	Au Rb
01-073-2899	I	Au Rb
04-003-1775	I	Au Rb
04-007-4057	S	Au Rb
00-026-0728	B	Ag Au S
03-065-8203	I	Ag Au Sb ₆

Alphabetical Formula Index Sort

Choose element:

- Au
- B
- Ba
- Be
- Bi
- Bk
- Br
- C
- Ca
- Cd

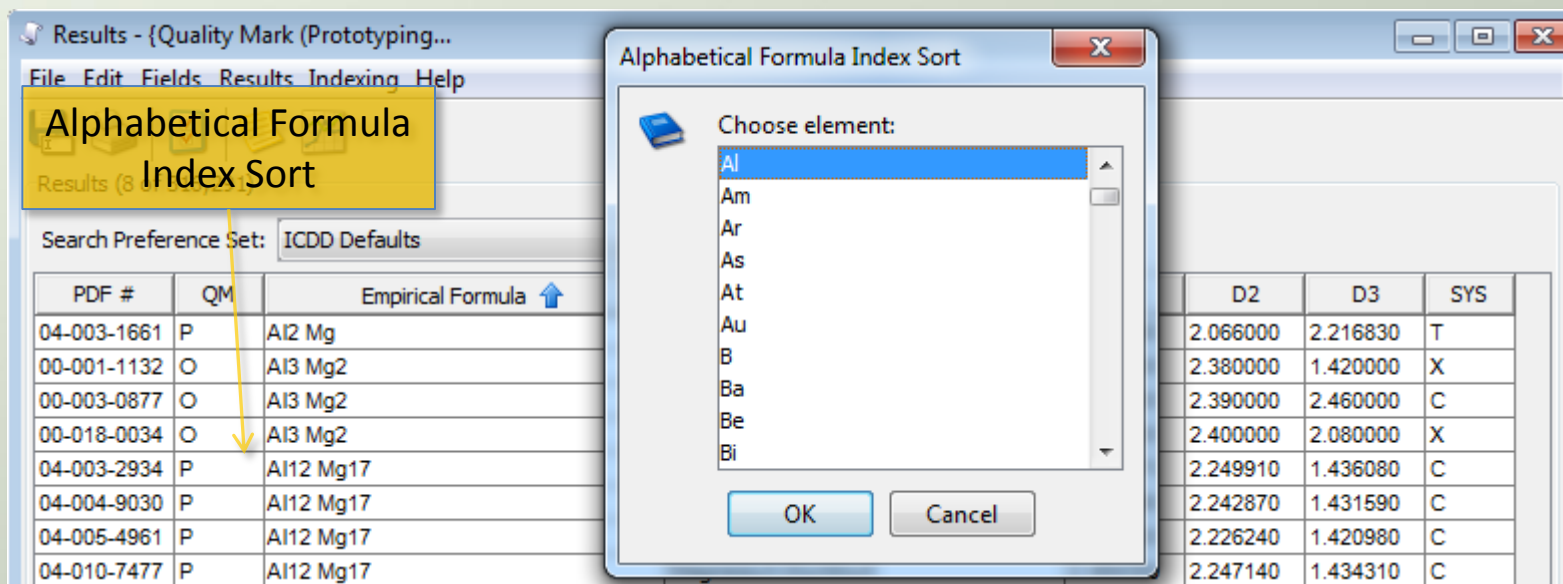
OK Cancel

	D2	D3	SYS
	1.673600	2.049000	C
	1.672100	1.094700	C
	1.669740	2.045000	C
	1.676680	2.053500	C
	1.673000	4.098000	C
	2.510000	1.770000	C
	2.111420	1.335380	C

Example 2

Alphabetical Formula Index Sort

- If 2 formulae elements are alphabetically equal and contain 2 or 3 elements, they are sorted by the ratio of the second-to-last divided by the last atomic weight from largest to smallest.
- Example 3: $\text{Al}_2 \text{Mg}$, $\text{Al}_3 \text{Mg}_2$, $\text{Al}_{12} \text{Mg}_{17}$ - sorted on **Al**
 - Since these are all alphabetically equivalent and are a binary system, they are sorted on their last 2 elements. The ratios are 2/1, 3/2, and 12/17. $\text{Al}_2 \text{Mg}$ is first because 2 is the larger than 3/2 and 12/17.
- Example 4: $\text{Al}_2 \text{Mg}_5 \text{Se}_8$, $\text{Al}_2 \text{Mg}_2 \text{Se}_5$ - sorted on **Al**
 - Since these are all alphabetically equivalent and are a ternary system, they are sorted on their last 2 elements. The ratios are 5/8, and 2/5. $\text{Al}_2 \text{Mg}_5 \text{Se}_8$ is first because 5/8 is the larger than 2/5.



The screenshot shows a software window titled 'Results - {Quality Mark (Prototyping...)' with a menu bar (File, Edit, Fields, Results, Indexing, Help). A yellow callout box highlights the 'Alphabetical Formula Index Sort' option. Below the menu is a search preference set for 'ICDD Defaults'. A table lists empirical formulas with columns for PDF #, QM, and Empirical Formula. A dialog box titled 'Alphabetical Formula Index Sort' is open, showing a list of elements with 'Al' selected. The dialog has 'OK' and 'Cancel' buttons. In the background, another table shows columns for D2, D3, and SYS with numerical values.

PDF #	QM	Empirical Formula
04-003-1661	P	Al ₂ Mg
00-001-1132	O	Al ₃ Mg ₂
00-003-0877	O	Al ₃ Mg ₂
00-018-0034	O	Al ₃ Mg ₂
04-003-2934	P	Al ₁₂ Mg ₁₇
04-004-9030	P	Al ₁₂ Mg ₁₇
04-005-4961	P	Al ₁₂ Mg ₁₇
04-010-7477	P	Al ₁₂ Mg ₁₇

D2	D3	SYS
2.066000	2.216830	T
2.380000	1.420000	X
2.390000	2.460000	C
2.400000	2.080000	X
2.249910	1.436080	C
2.242870	1.431590	C
2.226240	1.420980	C
2.247140	1.434310	C

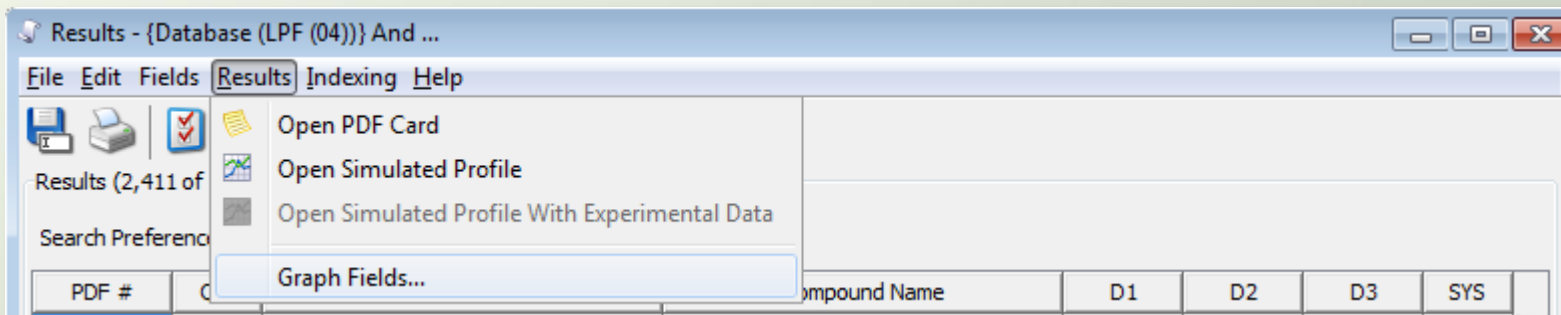
Example 3

Alphabetical Formula Index Sort

- If formulae elements are alphabetically equivalent and higher than a ternary system, atomic weights are sorted alphabetically.
- Example 5: Nb **S** Se₂ Sn, Nb **S** Se₂ Sn_{0.50} - sorted on **S**
 - Since these are all alphabetically equivalent and are higher than a ternary system, they are sorted by their atomic weights alphabetically starting with the sort element. The first difference in atomic weight is Sn. Even though there is 1 Sn implied, it is not written and Nb S Se₂ Sn is listed first.

Graphing

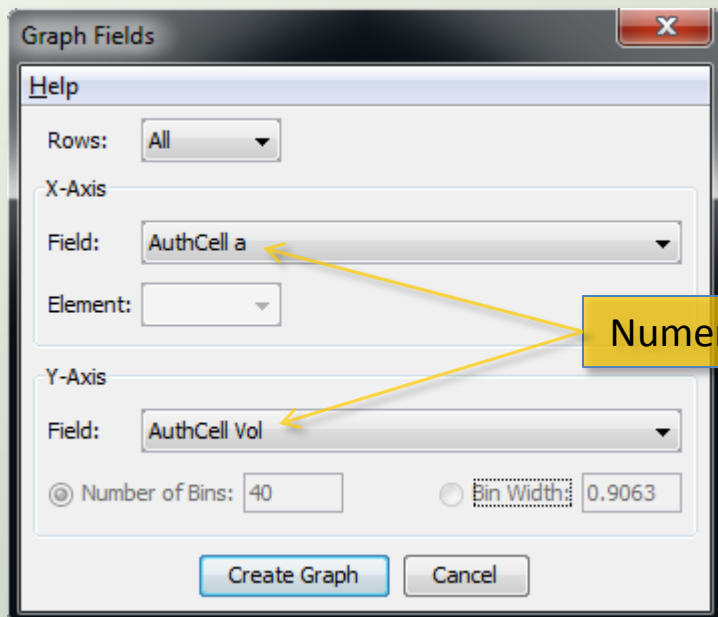
- The Results table can be graphed using any display field.
- To graph a field, click the Results menu and select *Graph Fields*.



- Depending on the display field(s) selected, there are three different types of graphs available:
 - X-Y graph
 - Histogram
 - Category graph

Graphing - X-Y Graph

- If the x-axis field and y-axis field are both numeric fields, then an X-Y graph will be displayed.
- You can limit the rows to be graphed by pre-selecting the rows in the Results table first. Otherwise, the graph will use all rows as indicated by the *Rows* selection box.



Graph Fields

Help

Rows: All

X-Axis
Field: AuthCell a

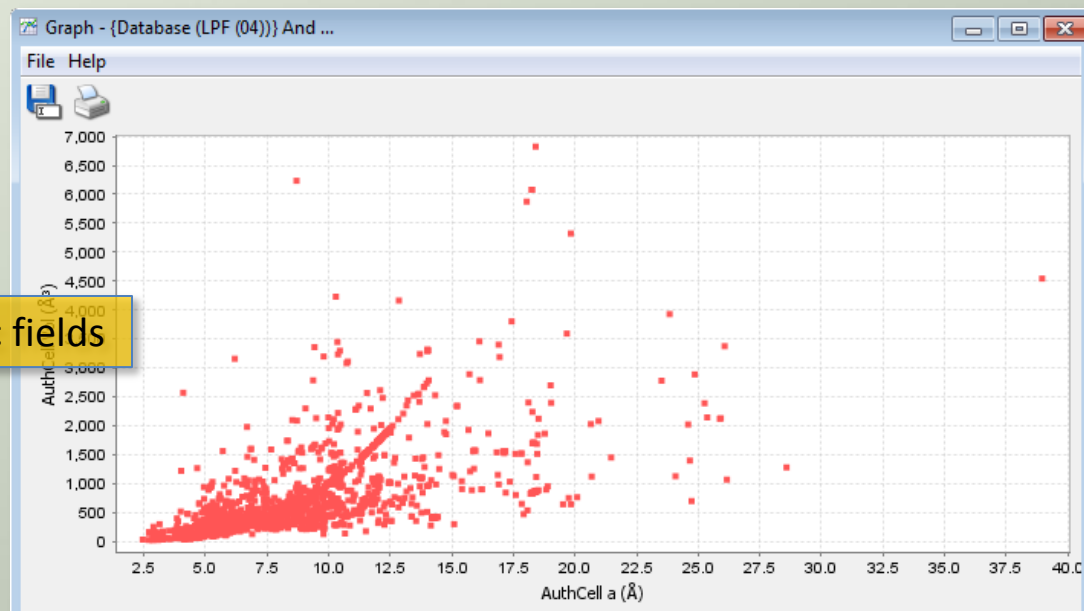
Element:

Y-Axis
Field: AuthCell Vol

Number of Bins: 40 Bin Width: 0.9063

Create Graph Cancel

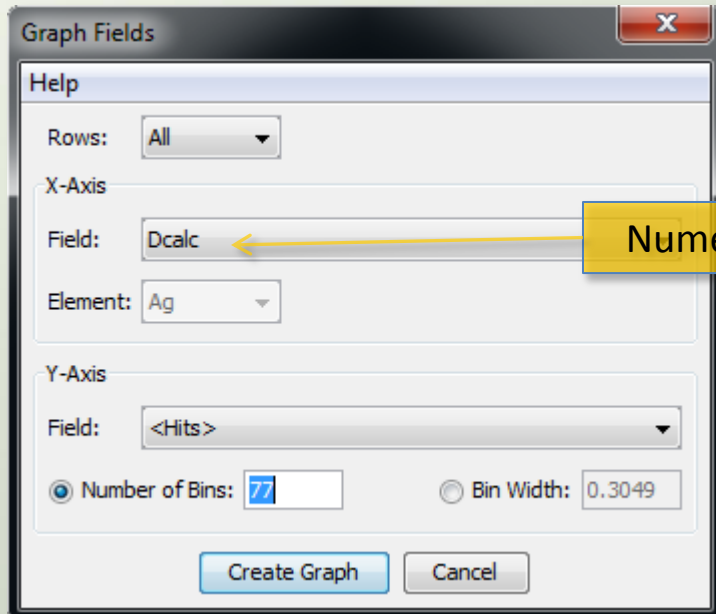
Graph Fields form



X-Y graph of author's cell volume and author's cell a

Graphing - Histogram

- If the x-axis field is a numeric field and the y-axis field is <Hits>, then a histogram will be displayed.
- Individual element values for the weight % and atomic % x-axis fields can be selected in the *Element* listbox.
- You can customize the histogram bin (bar) distribution by changing the *Number of Bins* or *Bin Width* values.



Graph Fields

Help

Rows: All

X-Axis

Field: Dcalc

Element: Ag

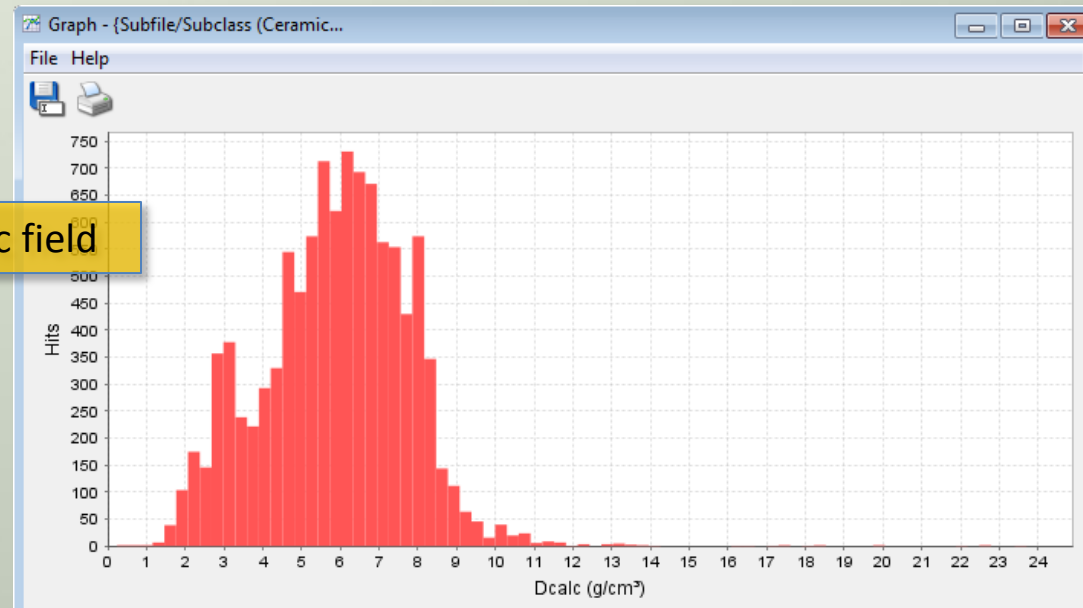
Y-Axis

Field: <Hits>

Number of Bins: 77 Bin Width: 0.3049

Create Graph Cancel

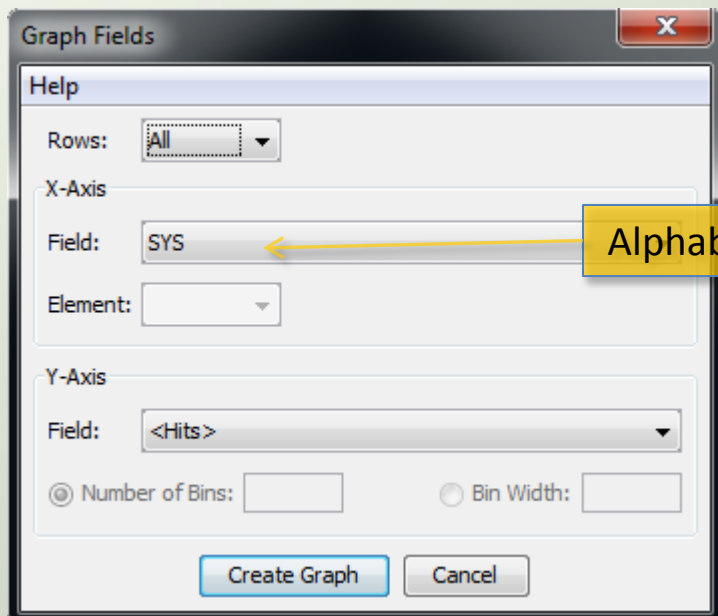
Graph Fields form



Histogram of the calculated densities for all ceramics

Graphing – Category Graph

- If the x-axis field is an alphabetic field, then a category graph will be displayed.
- The y-axis field will default to <Hits>, indicating that the y-axis represents the number of entries for each unique x-axis value (category).



Graph Fields

Help

Rows: All

X-Axis
Field: SYS

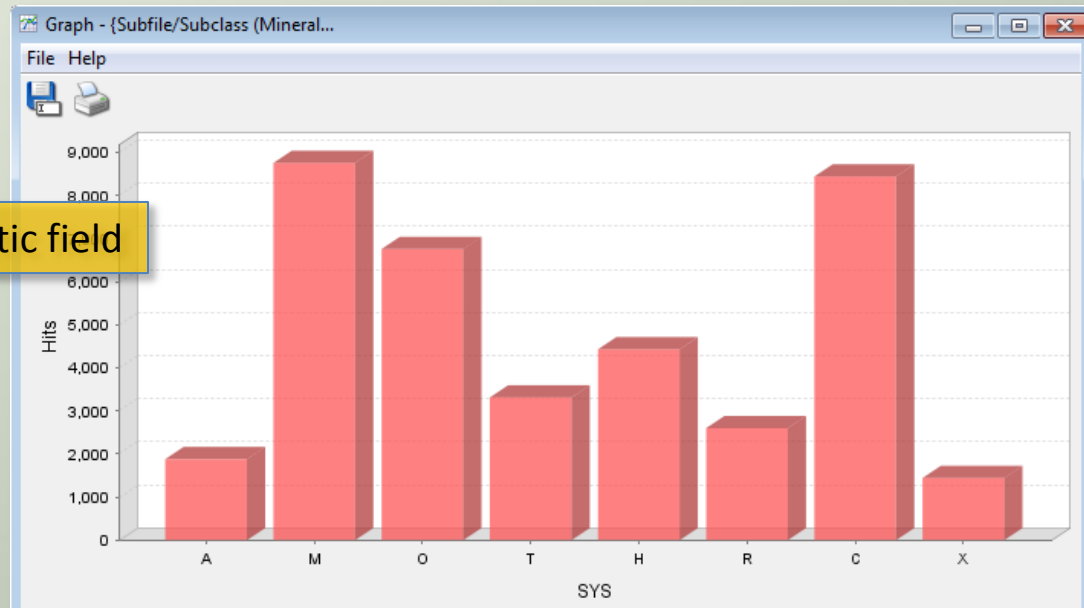
Element:

Y-Axis
Field: <Hits>

Number of Bins: Bin Width:

Create Graph Cancel

Graph Fields form



Category graph of the crystal system distribution for all minerals



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

www.icdd.com

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