

Sort, Order and Graph Data

Sort and Order

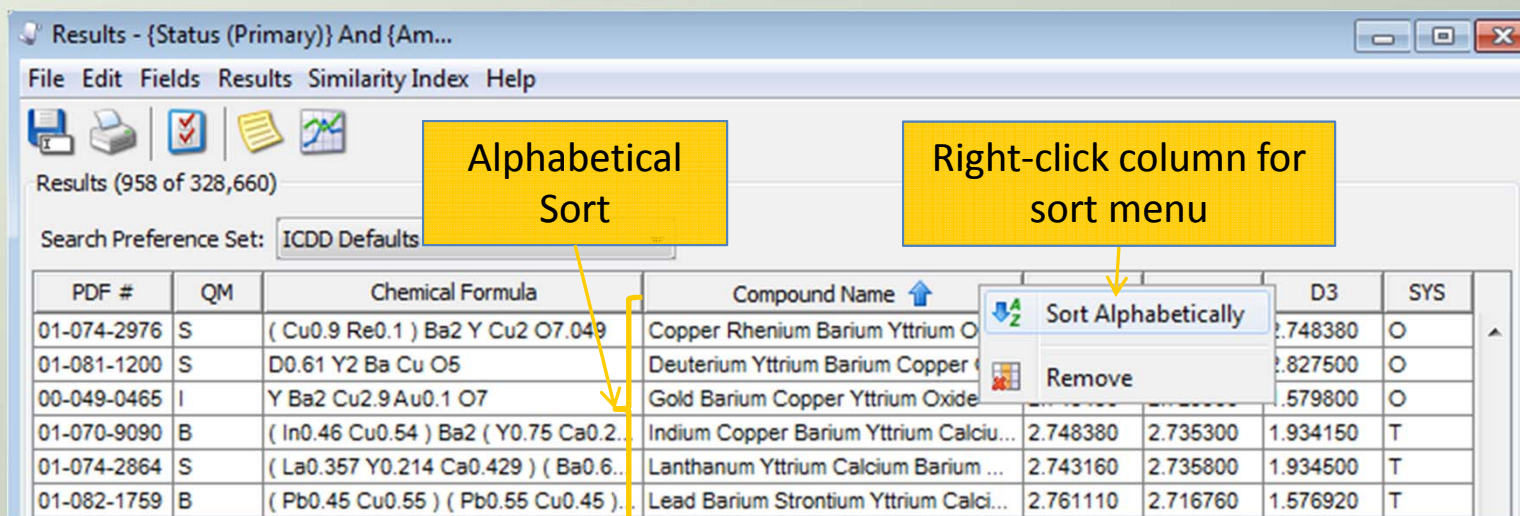
- What?
 - Sorting is the ability to order the PDF data retrieved from the search results.
- Why?
 - To organize the data.
 - To find relevant data faster and easier.
- How?
 - Use the Results table.

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 - {Status (Primary)} And {Am...}

File Edit Fields Results Similarity Index Help

Results (958 of 328,660)

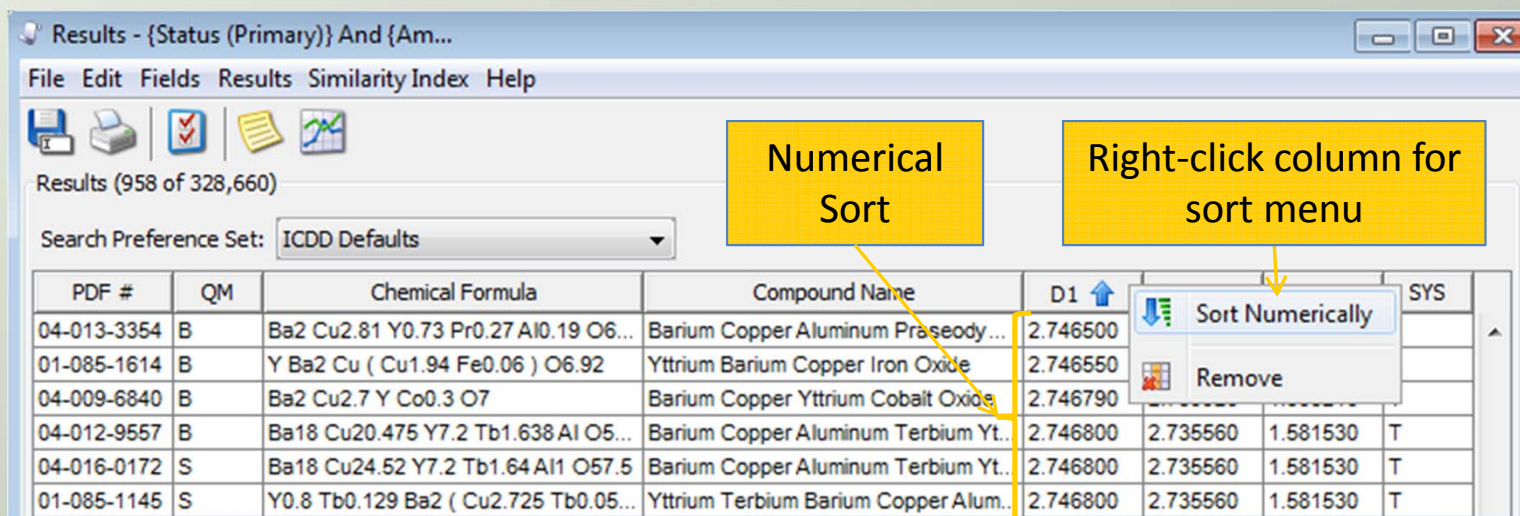
Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D3	SYS
01-074-2976	S	(Cu0.9 Re0.1) Ba2 Y Cu2 O7.049	Copper Rhenium Barium Yttrium O...	2.748380	O
01-081-1200	S	D0.61 Y2 Ba Cu O5	Deuterium Yttrium Barium Copper	2.827500	O
00-049-0465	I	Y Ba2 Cu2.9 Au0.1 O7	Gold Barium Copper Yttrium Oxide	1.579800	O
01-070-9090	B	(In0.46 Cu0.54) Ba2 (Y0.75 Ca0.2...	Indium Copper Barium Yttrium Calciu...	2.748380	2.735300
01-074-2864	S	(La0.357 Y0.214 Ca0.429) (Ba0.6...	Lanthanum Yttrium Calcium Barium ...	2.743160	2.735800
01-082-1759	B	(Pb0.45 Cu0.55) (Pb0.55 Cu0.45)	Lead Barium Strontium Yttrium Calci...	2.761110	2.716760

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 - {Status (Primary)} And {Am...}

File Edit Fields Results Similarity Index Help

Results (958 of 328,660)

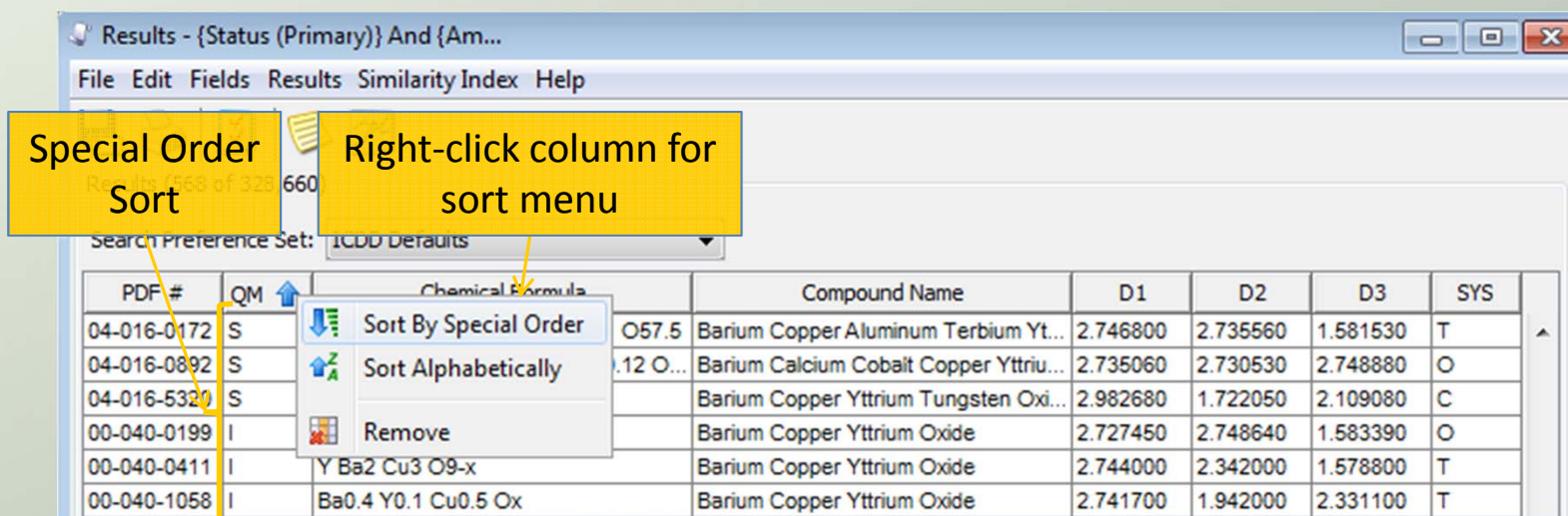
Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D1 ↑				SYS
04-013-3354	B	Ba2 Cu2.81 Y0.73 Pr0.27 Al0.19 O6...	Barium Copper Aluminum Praseody...	2.746500				
01-085-1614	B	Y Ba2 Cu (Cu1.94 Fe0.06) O6.92	Yttrium Barium Copper Iron Oxide	2.746550				
04-009-6840	B	Ba2 Cu2.7 Y Co0.3 O7	Barium Copper Yttrium Cobalt Oxide	2.746790				
04-012-9557	B	Ba18 Cu20.475 Y7.2 Tb1.638 Al O5...	Barium Copper Aluminum Terbium Yt...	2.746800	2.735560	1.581530		T
04-016-0172	S	Ba18 Cu24.52 Y7.2 Tb1.64 Al O57.5	Barium Copper Aluminum Terbium Yt...	2.746800	2.735560	1.581530		T
01-085-1145	S	Y0.8 Tb0.129 Ba2 (Cu2.725 Tb0.05...	Yttrium Terbium Barium Copper Alum...	2.746800	2.735560	1.581530		T

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), R (Rietveld), I (Indexed), C (Calculated), B (Blank), O (Low-Precision), P (Prototyping), H (Hypothetical), G (Good), M (Minimal Acceptable)
 - Descending: M (Minimal Acceptable), G (Good), H (Hypothetical), P (Prototyping), O (Low-Precision), B (Blank), C (Calculated), I (Indexed), R (Rietveld), S (Star)



Results - {Status (Primary)} And {Am...}

File Edit Fields Results Similarity Index Help

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
04-016-0172	S	O57.5	Barium Copper Aluminum Terbium Yt...	2.746800	2.735560	1.581530	T
04-016-0892	S	12 O...	Barium Calcium Cobalt Copper Yttri...	2.735060	2.730530	2.748880	O
04-016-5320	S		Barium Copper Yttrium Tungsten Oxi...	2.982680	1.722050	2.109080	C
00-040-0199	I		Barium Copper Yttrium Oxide	2.727450	2.748640	1.583390	O
00-040-0411	I	Y Ba ₂ Cu ₃ O _{9-x}	Barium Copper Yttrium Oxide	2.744000	2.342000	1.578800	T
00-040-1058	I	Ba _{0.4} Y _{0.1} Cu _{0.5} O _x	Barium Copper Yttrium Oxide	2.741700	1.942000	2.331100	T

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 Similarity Index Help

Results (12 of 328,660)

Search Preference Set: ICDD Defaults

PDF #	QM	Chemical Formula	Compound Name	SYS	D1	D2	D3
00-050-0835	S	Hg _{1.24} Ti S ₂	Mercury Titanium Sulfide	M			00
01-087-1124	S	Rb _{0.48} V ₂ O ₅	Rubidium Vanadium Oxide	M			70
00-038-1235	S	K Hg C ₄	Potassium Mercury Carbide	O			00
00-051-0656	S	Li ₃ C ₈	Lithium Graphite	H			40
00-055-1157	S	C ₆₀ · 2 C H Br ₃	Fullerene bromoform	H	4.572010	4.419550	6.692790
01-088-1596	S	Sn Ta S ₂	Tin Tantalum Sulfide	H	4.358100	2.719570	2.039080

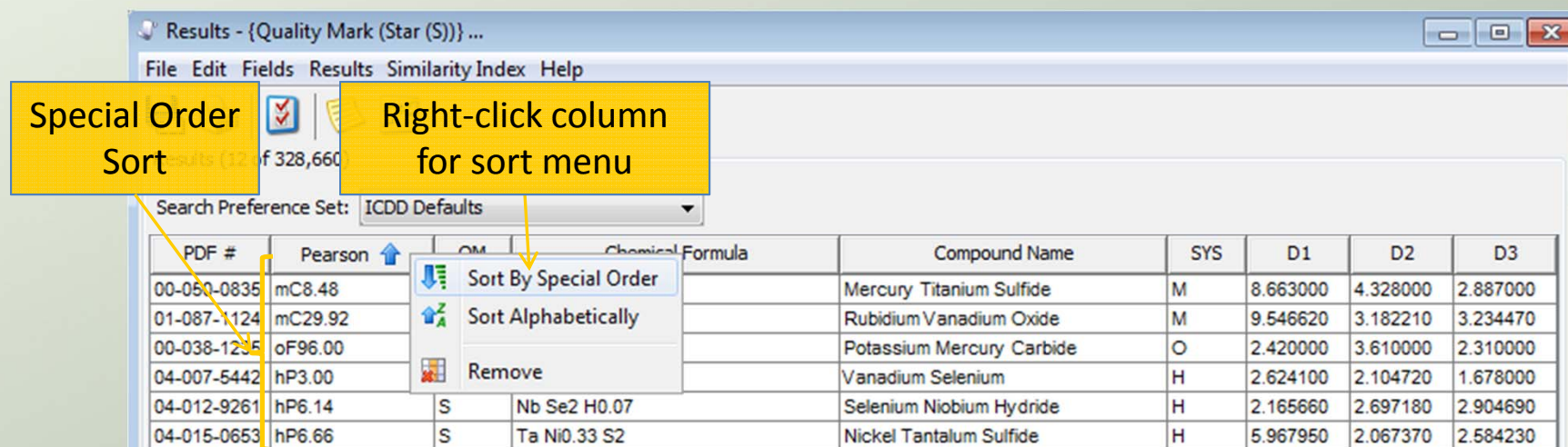
Sorted by SYS (Crystal System)

Special Order
Sort

Right-click column for
sort menu

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 Similarity Index Help

Search Preference Set: ICDD Defaults

PDF #	Pearson	OM	Chemical Formula	Compound Name	SYS	D1	D2	D3
00-050-0835	mC8.48			Mercury Titanium Sulfide	M	8.663000	4.328000	2.887000
01-087-1124	mC29.92			Rubidium Vanadium Oxide	M	9.546620	3.182210	3.234470
00-038-1255	oF96.00			Potassium Mercury Carbide	O	2.420000	3.610000	2.310000
04-007-5442	hP3.00			Vanadium Selenium	H	2.624100	2.104720	1.678000
04-012-9261	hP6.14	S	Nb Se ₂ H _{0.07}	Selenium Niobium Hydride	H	2.165660	2.697180	2.904690
04-015-0653	hP6.66	S	Ta Ni _{0.33} S ₂	Nickel Tantalum Sulfide	H	5.967950	2.067370	2.584230

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 Similarity Index Help

Alphabetical Formula Index Sort

Search Preference Set: ICDD Defaults

PDF #	QM	Empirical Formula	
00-034-1047	I	Au Rb	Gold F
00-050-1036	C	Au Rb	Gold F
01-073-2899	I	Au Rb	Gold F
04-003-1775	I	Au Rb	Gold F
04-007-4057	S	Au Rb	Gold F
00-019-1146	O	Ag Au S	Gold S
00-026-0728	B	Ag Au S	Gold S
00-038-0396	B	Ag Au S	Gold S
03-065-8203	I	Ag Au Sb ₆	Silver Gold Antimony

Choose element:

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

OK Cancel

D2	D3
73600	2.049000
72100	1.094700
69740	2.045000
76680	2.053500
73000	4.098000
30000	2.390000
10000	1.770000
30000	2.390000

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: **Al₂ Mg**, **Al₃ Mg₂**, **Al₁₂ Mg₁₇** - 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. **Al₂ Mg** is first because 2 is the larger than 3/2 and 12/17.
- Example 4: **Al₂ Mg₅ Se₈**, **Al₂ Mg₂ Se₅** - 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. **Al₂ Mg₅ Se₈** is first because 5/8 is the larger than 2/5.

Results - {Empirical Formula Exactly...}

Alphabetical Formula Index Sort

Search Preference Set: ICDD Defaults

PDF #	QM	Empirical Formula	
00-003-0876	B	Al ₂ Mg	Aluminum
00-034-1035	B	Al ₂ Mg	Aluminum
04-003-1661	P	Al ₂ Mg	Aluminum
00-040-0903	B	Al ₃ Mg ₂	Aluminum
00-001-1128	B	Al ₁₂ Mg ₁₇	Aluminum
04-003-2934	P	Al ₁₂ Mg ₁₇	Aluminum
04-004-9030	P	Al ₁₂ Mg ₁₇	Aluminum
04-005-4961	P	Al ₁₂ Mg ₁₇	Aluminum
04-010-7477	P	Al ₁₂ Mg ₁₇	Aluminum Magnesium

Alphabetical Formula Index Sort

Choose element:

- Al
- Am
- Ar
- As
- At
- Au
- B
- Ba
- Be
- Bi

OK Cancel

	D3
00	2.210000
00	2.440000
00	2.216830
00	2.200000
00	1.430000
10	1.436080
70	1.431590
40	1.420980
	1.434310

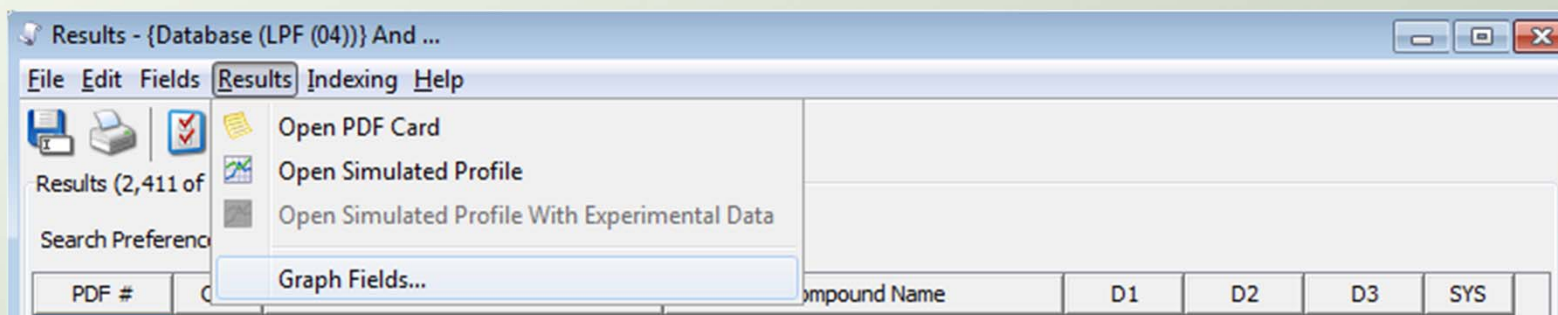
Example 3

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

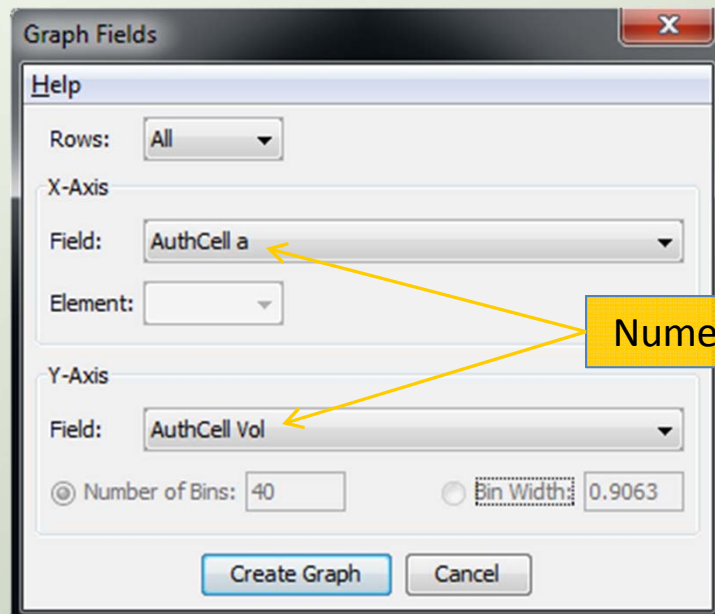
- The Results table can be graphed using any display field.
- To graph a field, click the Results menu and select *Graph Fields*.



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

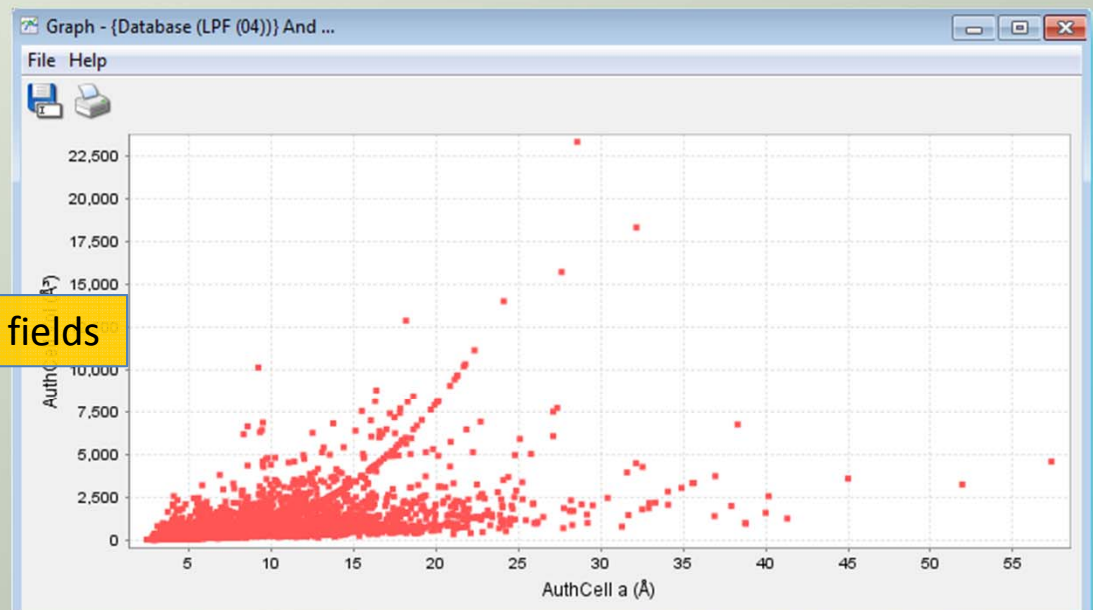
Graphing - X-Y Graph

- 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.



The 'Graph Fields' dialog box is shown. It has a 'Help' tab. Under 'Rows', a dropdown menu is set to 'All'. Under 'X-Axis', the 'Field' dropdown is set to 'AuthCell a' and the 'Element' dropdown is empty. Under 'Y-Axis', the 'Field' dropdown is set to 'AuthCell Vol'. At the bottom, there are two options: 'Number of Bins' (set to 40) and 'Bin Width' (set to 0.9063). There are 'Create Graph' and 'Cancel' buttons at the bottom.

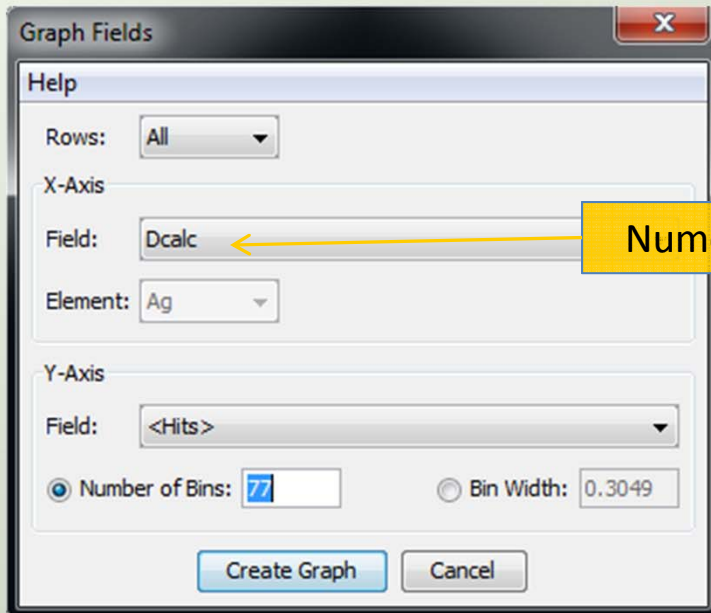
Graph Fields form



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

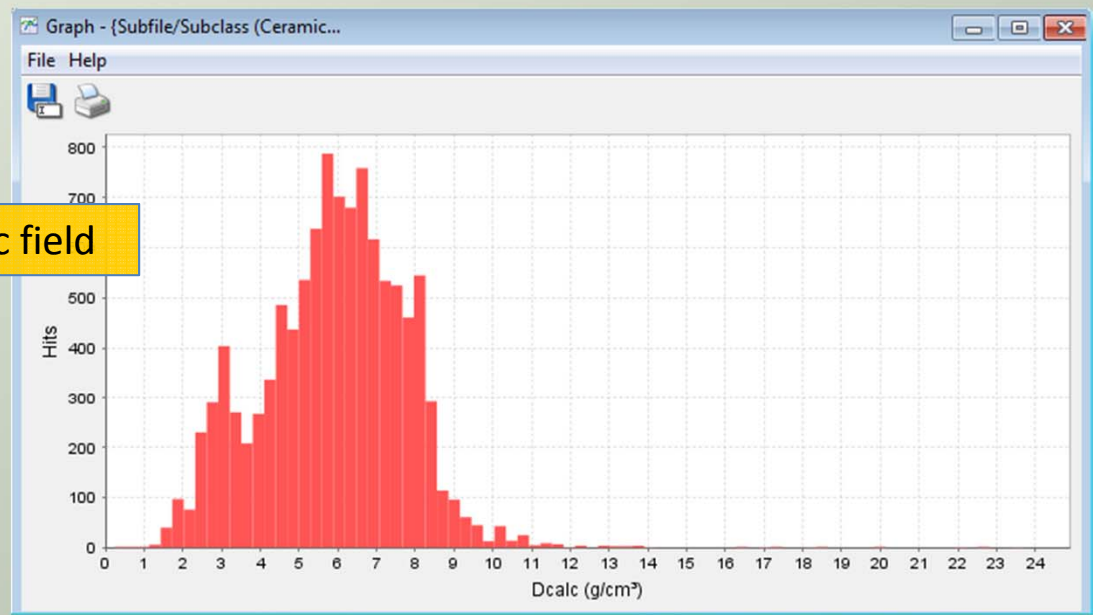
Graphing - Histogram

- 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.



The 'Graph Fields' dialog box is shown. It has a 'Help' tab. Under 'X-Axis', the 'Field' is set to 'Dcalc' and the 'Element' is set to 'Ag'. Under 'Y-Axis', the 'Field' is set to '<Hits>'. At the bottom, there are two options: 'Number of Bins' (set to 77) and 'Bin Width' (set to 0.3049). There are 'Create Graph' and 'Cancel' buttons at the bottom right.

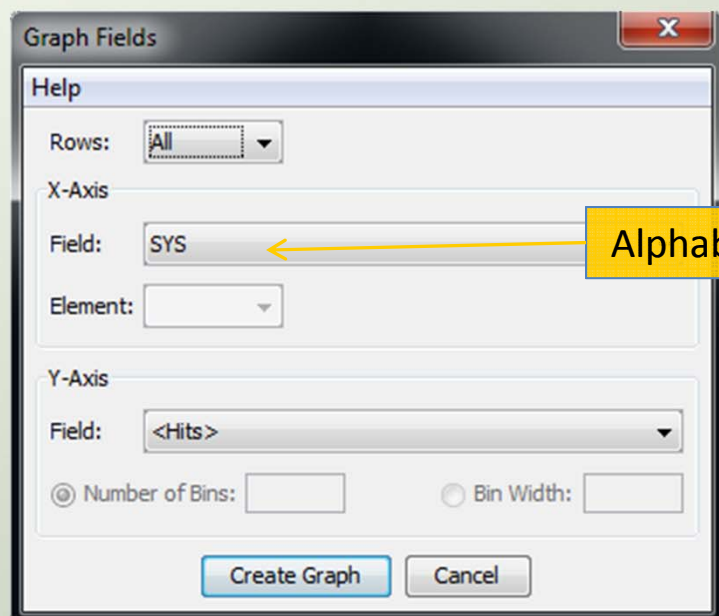
Graph Fields form



Histogram of the calculated densities for all ceramics

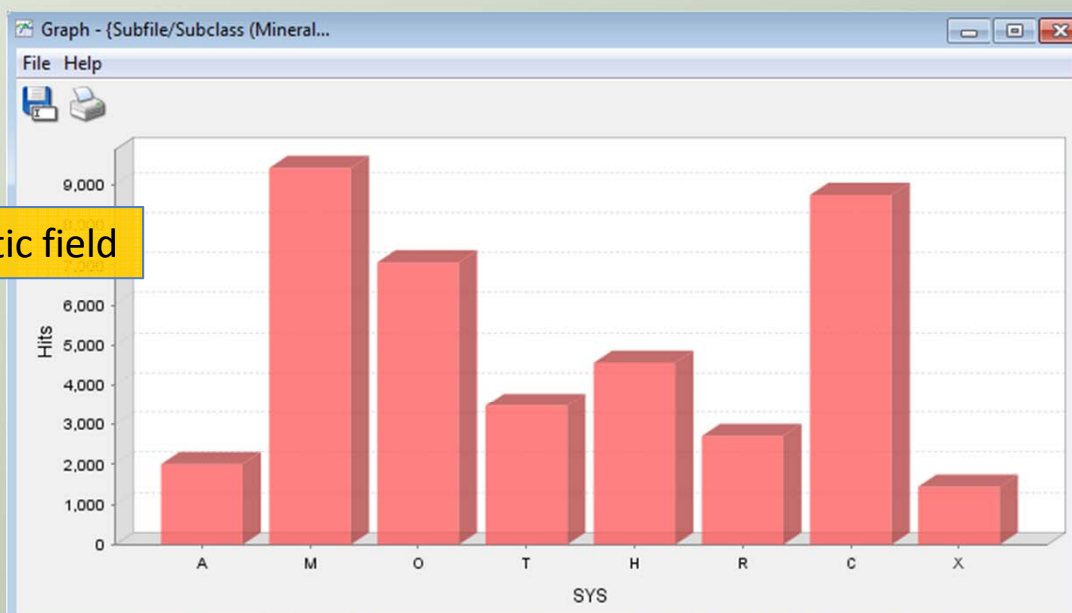
Graphing – Category Graph

- 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).



The 'Graph Fields' dialog box is shown. It has a 'Help' tab. Under 'X-Axis', the 'Field' is set to 'SYS' and 'Element' is empty. Under 'Y-Axis', the 'Field' is set to '<Hits>'. There are radio buttons for 'Number of Bins' and 'Bin Width', both with empty input fields. 'Create Graph' and 'Cancel' buttons are at the bottom.

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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