

# New Release Features

# New Release Features

- The 2011 release of ICDD databases boasts an impressive array of new features. This tutorial will show these new features using ICDD's own data-mining software, which is bundled free with the database. These features include:
  - Enhanced searching
  - Revamped user interfaces
  - Modulated structures
  - Improved Sleve+ functionality

# New Search and Display Field: Structural Formula\*

Search

Global Operator Numeric Input Help

References Structures Miscellaneous  
Subfiles/Database Filters Periodic Table Elements Names

**Structural Formula**

Not Contains Phrase Cu Cl2

Empirical Formula

Not Contains Elements

Formula Type (ANX)

Not Contains Phrase

Composition (1)

Not  Weight %  Atomic %

El.	Value	ESD

Number of Elements (# El's)

Not

1  Or

2

3

4

5

6

7

8

9

>=10

Search  Show Results  Undock Page

Structural Formula search

Results - {Structural Formula Contain...}

File Edit Fields Results Indexing

Results (43 of 316,291)

Search Preference Set: ICDD Defaults

PDF #	Structural Formula	Compound Name	SYS
00-006-0049	N H ( C H2 C H2 N H2 )2 · Cu Cl2 · 0.5...	Diethylenetriamine copper chloride he...	M
00-019-1795	C H3 O H · Cu Cl2	Copper methanol chloride	X
00-019-1797	C2 H6 ( O H )2 · Cu Cl2	Copper dimethanol chloride	X
00-021-1591	Cu Cl2 · 2 ( C2 H5 )2 N H	Copper chloride bis(diethylamine)	X
00-021-1594	Cu Cl2 · 4 C2 H5 N H2	Copper chloride tetrakis(ethylamine)	X
00-021-1595	Cu Cl2 · 2 C2 H5 N H2	Copper chloride bis(ethylamine)	X
00-022-0120	Cu Cl2 · Cd Cl2 · 4 H2 O	Cadmium Copper Chloride Hydrate	M
00-022-0228	( Cu Cl2 · B N )	Copper Boron Chloride Nitride	X
00-022-0602	Cu Cl2 · 1.50 C H3 C O O H	Copper Hydrogen Chloride Acetate	X
00-023-0953	2 Cu Cl2 · Cu ( O H )2	Copper Chloride Hydroxide	X
00-024-0353	2 Cu Cl2 · Cu ( O H )2 · 2 H2 O	Copper Chloride Hydroxide Hydrate	A
00-024-1335	2 Cs Cl · Cu Cl2	Cesium Copper Chloride	O
00-025-0262	Cu Cl2 · 2 N H4 Cl · 2 H2 O	Ammonium Copper Chloride Hydrate	T
00-026-0065	2 N H4 Cl · Cu Cl2	Ammonium Copper Chloride	O
00-027-1603	Cu Cl2 ( ( C2 H5 )2 N C H2 )2	Copper tetraethylethylene diamine chl...	M
00-030-1631	Cu Cl2 ( C12 H8 N2 O )2 · 2 H2 O	Copper bis(phenanthroline N-oxide) c...	X
00-030-1647	Cu Cl2 ( C3 H4 N2 )2	Copper dichloro bis(pyrazole)	A
00-034-1903	Cu Cl2 C21 H27 O2 N · 2 H2 O	Copper chloride diethylaminopropiony...	X
00-041-1522	( C10 H8 N2 O )2 Cu Cl2	Copper 2,2'-dipyridyl-2-N-oxide chloride	X
00-044-1567	( C7 H7 N5 ) Cu Cl2 · 2 H2 O	Copper 3-amino-5-(2-pyridyl)-1,2,4-tri...	X
00-044-1569	( C12 H13 N3 O2 )2 Cu Cl2	Copper bis(2-aminoacetophenone 2-f...	X

Search Description: {Structural Formula Contains Phrase 'Cu Cl2'}

Calculations: Mean:  Median:  ESD:

Patterns with a Structural Formula containing "Cu Cl2"

# New Search: Property Sheet\*

Property Sheets contains an Adobe PDF of battery material or ionic conductor information

Property Sheet - Ce Co3 - 04-004-1681

File View Document Help

Page 1 of 2

**Hydrogenation-dehydrogenation properties of IMC P-C-T isotherms for CeCo<sub>3</sub>-H<sub>2</sub> system**

*Parent Compound:*  
 Chemical name: Cerium Cobalt  
 Chemical formula: CeCo<sub>3</sub>  
 Crystal structure: *R*-3*m*, *a*= 4.955, *c*= 24.75 [1]  
 Powder Pattern: 00-020-0263; 01-074-8422; 04-001-351595; 04-004-0584; 04-004-1370; 04-004-1433; 04-008-5852; 04-012-7500.

*Hydride:*  
 Chemical name: Cerium Cobalt Hydride  
 Chemical formula: CeCo<sub>3</sub>H<sub>4</sub>  
 Crystal structure: *R*-3*m*, *a*= 4.929; *c*=32.58 [2]  
 Powder Pattern: -

Alloy was obtained from pure metals by elect atmosphere with sequential quenching for 240 h a investigation of the interaction of compounds with hyc apparatus under a pressure of hydrogen to 2000 isotherms of hydrogen for the investigated compound 50°C and -70°C and under pressure to 2000 atm. are p

Analyses of the absorption-desorption isotherms high pressure shows that over the whole interval o absorption of hydrogen at room temperatures. There w of the hydride phase from CeCo<sub>3</sub>H<sub>4.5</sub> to CeCo<sub>3</sub>H<sub>6.1</sub> wi 40 to 1730 atm. at this temperature. Desorption of hyc up to 70 atm. leads to the formation of a hydride p CeCo<sub>3</sub>H<sub>4.9</sub>.

Absorption of hydrogen at low temperature (-70°C) leads to the formation of a hydride with the com

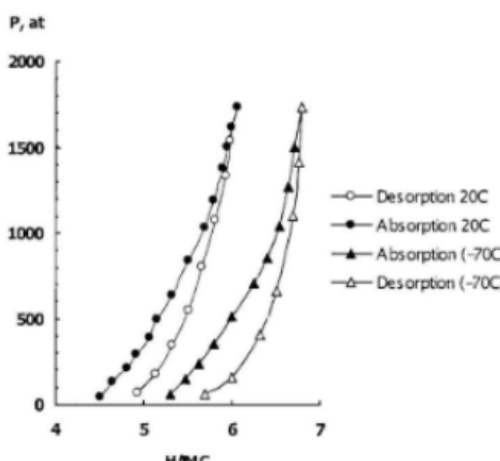
Cross-Ref PDF #'s (10)  
 00-020-0263 (Primary)  
 ✓ 04-001-3508 (Alternate)  
 ✓ 04-002-9552 (Alternate)  
 ✓ 04-003-1595 (Alternate)  
 ✓ 04-004-0584 (Alternate)  
 ✓ 04-004-1370 (Alternate)  
 ✓ 04-004-1433 (Alternate)  
 ✓ 04-005-4941 (Alternate)  
 ✓ 04-008-5852 (Alternate)  
 ✓ 04-012-7500 (Primary)

First page of Property Sheet for Cerium Cobalt

Property Sheet - Ce Co3 - 04-004-1681

File View Document Help

Page 2 of 2



absorption-desorption isotherms of hydrogen in the CeCo<sub>3</sub>-H<sub>2</sub>[3]

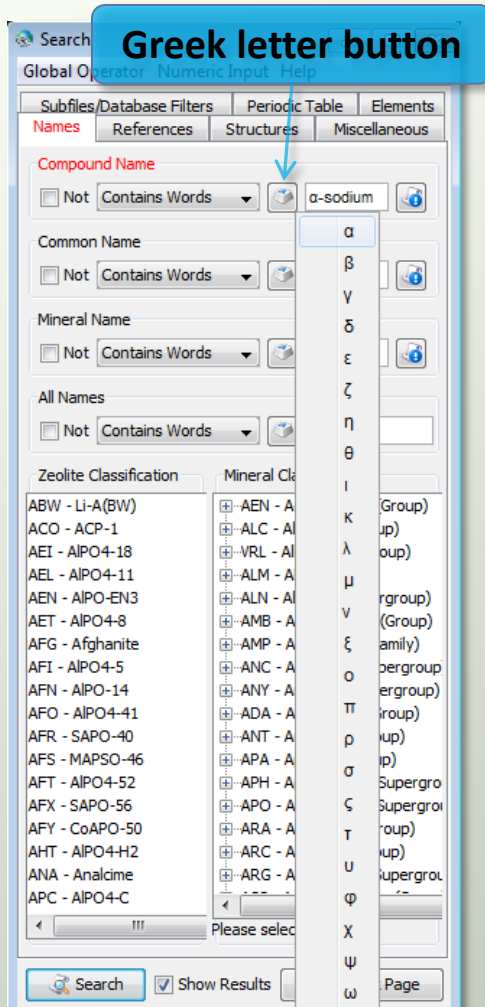
en R.H., Buschow K.H.J. Journal of the Less-Common Met 198.  
 /A., Burnasheva V.V., Semenenko K.N., Fadeeva N.V., Sol Journal of Hydrogen Energy. Oxford, 7(12) (1982) 957-96  
 kov S.A., Klyamkin S.N., Verbetsky V.N. Journal of 330-332 (2002) 574-578.

Cross-Ref PDF #'s (10)  
 00-020-0263 (Primary)  
 ✓ 04-001-3508 (Alternate)  
 ✓ 04-002-9552 (Alternate)  
 ✓ 04-003-1595 (Alternate)  
 ✓ 04-004-0584 (Alternate)  
 ✓ 04-004-1370 (Alternate)  
 ✓ 04-004-1433 (Alternate)  
 ✓ 04-005-4941 (Alternate)  
 ✓ 04-008-5852 (Alternate)  
 ✓ 04-012-7500 (Primary)

Second page of Property Sheet for Cerium Cobalt

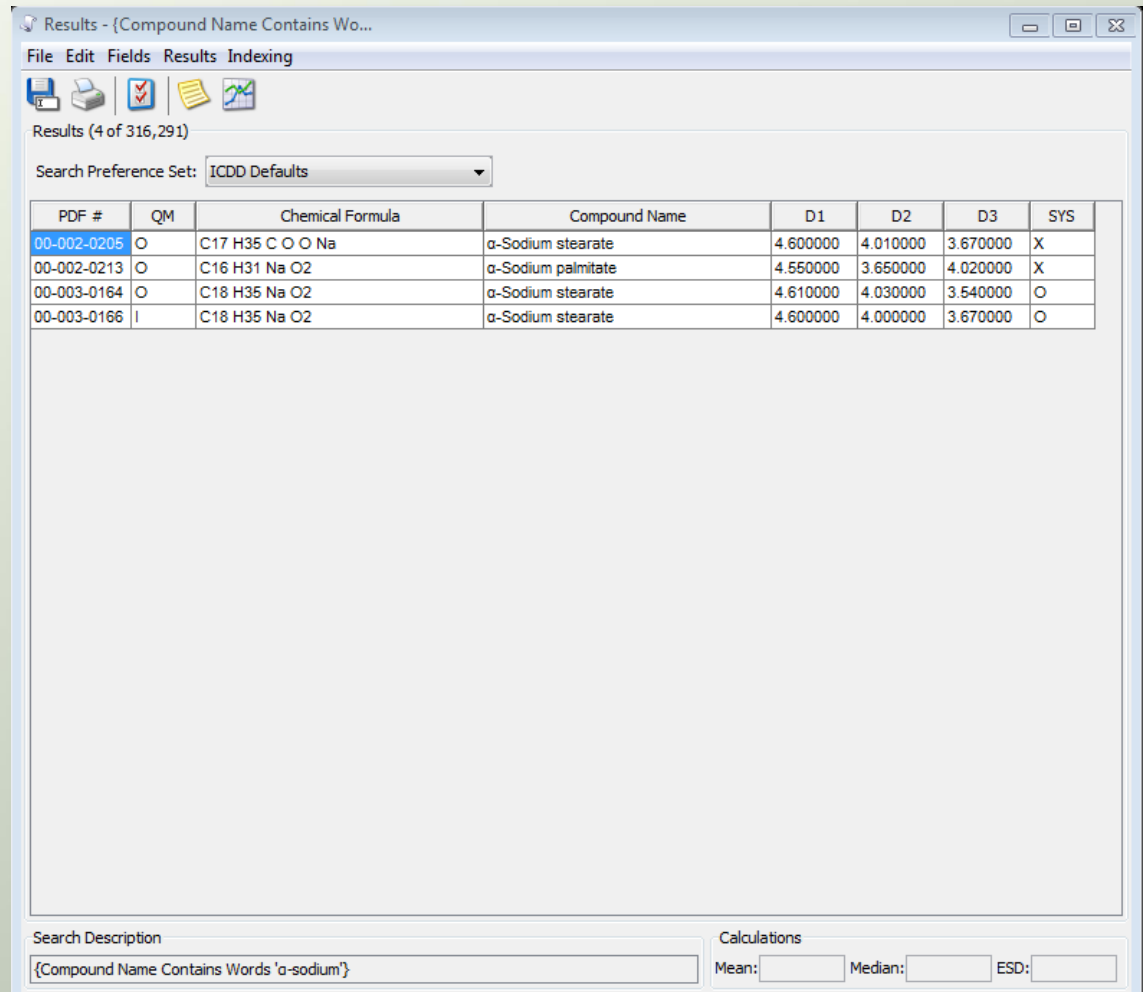
# Greek Letter Searches

Many of the fields in the database contain Greek letters. A new Greek letter button has been added, allowing the user to conveniently insert Greek letters for searching.



The screenshot shows the search interface with a blue callout box highlighting the 'Greek letter button' (a small icon of a Greek letter alpha) next to the search criteria 'α-sodium'. The interface includes sections for 'Compound Name', 'Common Name', 'Mineral Name', and 'All Names', each with a 'Contains Words' dropdown and a button. A 'Zeolite Classification' list is visible on the left, and a 'Mineral Classification' list is on the right.

*Popup list for inserting Greek letters*



The screenshot shows the search results window titled 'Results - {Compound Name Contains Wo...'. The search criteria is 'α-sodium'. The results table displays the following data:

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
00-002-0205	O	C17 H35 C O O Na	α-Sodium stearate	4.600000	4.010000	3.670000	X
00-002-0213	O	C16 H31 Na O2	α-Sodium palmitate	4.550000	3.650000	4.020000	X
00-003-0164	O	C18 H35 Na O2	α-Sodium stearate	4.610000	4.030000	3.540000	O
00-003-0166	I	C18 H35 Na O2	α-Sodium stearate	4.600000	4.000000	3.670000	O

The search description at the bottom is '{Compound Name Contains Words 'α-sodium'}'. The calculations section shows Mean, Median, and ESD fields.

*Results for the Compound Names containing "α-sodium"*

## “Yes/No/Maybe” Periodic Table Search

This new search option provides the user with a simpler way of mining the database for their search elements. For this search, an element can have one of three states.

The screenshot shows the ICDD Search interface with the following details:

- Search Box:** Contains the text "Yes/No/Maybe".
- Boolean Expression:** "Yes (H) No (All other elements) Maybe (C, N, O)".
- Search Results:**
  - Yes (White):** Elements H, Li, Na, K, Ca, Sc, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Rn.
  - No (Grey):** Elements U, Np, Am, Cm.
  - Maybe (Colored):** Elements He, Ne, Ar, Kr, Br, Rn, and elements C, N, O, F, Si, P, S, Cl, Al, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Ga, Ge, As, Se, Br, Kr, Xe, Rn.
- Callouts:**
  - Yes:** This element must exist in the pattern (white).
  - No:** This element must not exist in the pattern (grey).
  - Maybe:** This element may exist in the pattern (colored).

Periodic table search with new “Yes/No/Maybe” element option

# New Search Subfiles

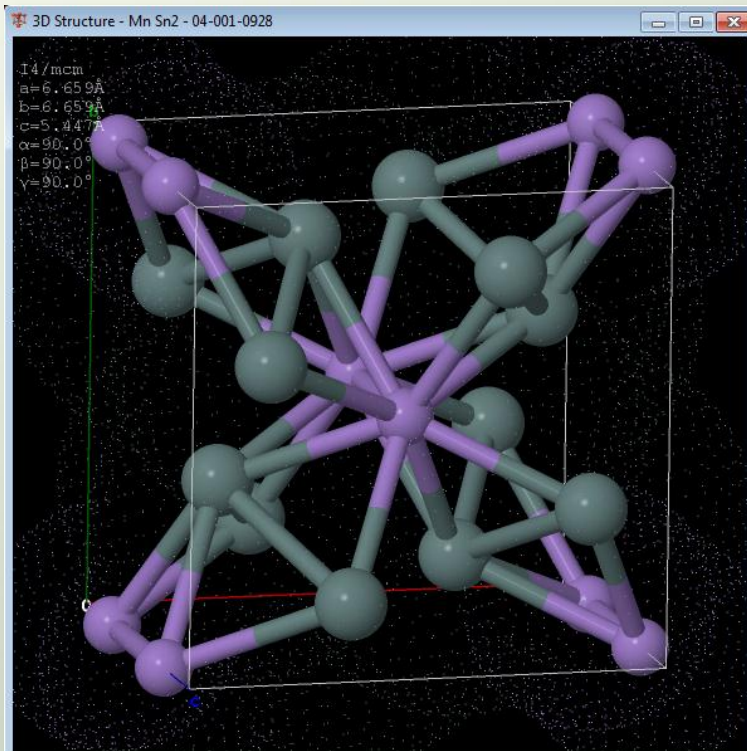
- Thermoelectric Material
- Modulated Structure
- Alkaloids\*
- Amino Acids, Peptides & Complexes\*
- Bioactivity\*
- Carbohydrate\*
- Merck\*
- Nucleosides & Nucleotides\*
- Porphyrins\*
- Steroids\*
- Terpenes\*

\*Subfile previously only available in PDF-4/Organics

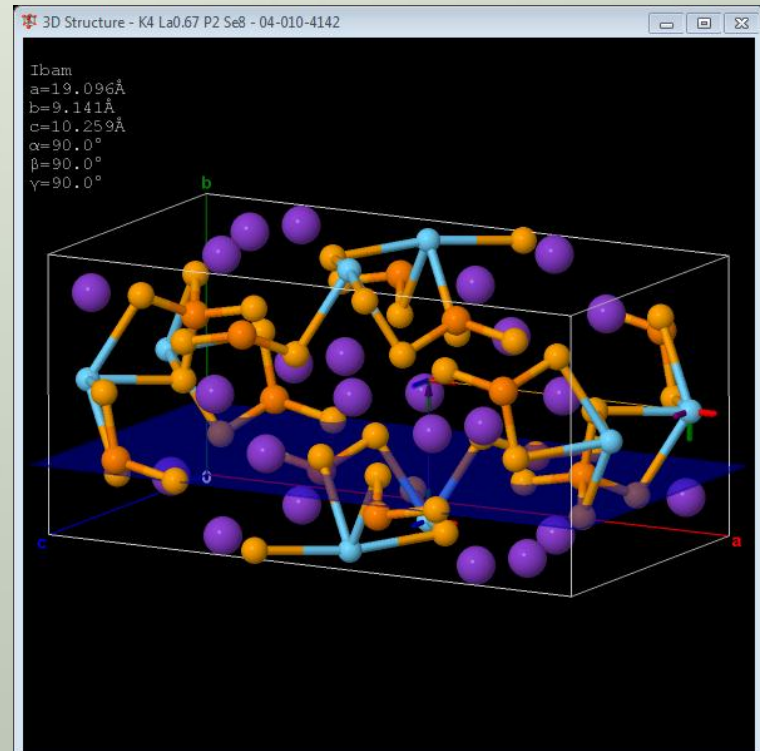
## Jmol – 3D Structure Viewer\*

We have upgraded the 3D structure viewer to use Jmol, a fast and powerful open-source structure viewer. Some of Jmol's features include:

- Dot surface, van der Waals surface, and molecular surface
  - Displaying individual symmetry operators
    - 3D stereographic viewing



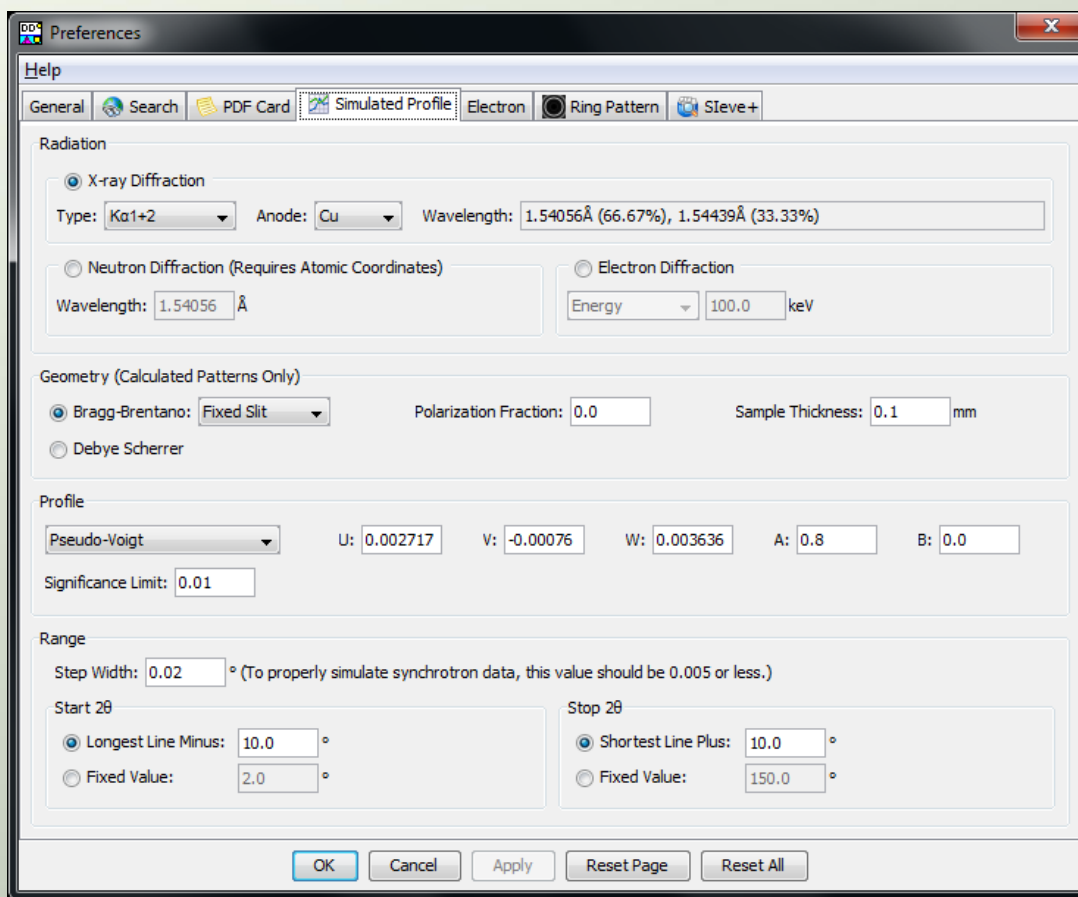
*3D structure for Manganese Tin with a dot surface overlay*



*3D structure for Potassium Lanthanum Phosphorus Selenide showing the a-glide plane symmetry operation*

## New Simulated Profile Preferences\*

We have merged the Experimental Pattern Preferences, Calculated Pattern Preferences, and Range Preferences into a unified Simulated Profile Preferences. Additionally, we have enabled the Crystallite Size profile function for experimental entries (previously only available for calculated entries).



**Preferences**

Help

General Search PDF Card **Simulated Profile** Electron Ring Pattern SIeve+

**Radiation**

X-ray Diffraction  
 Type:  Anode:  Wavelength:

Neutron Diffraction (Requires Atomic Coordinates) Wavelength:  Å

Electron Diffraction Energy:  keV

**Geometry (Calculated Patterns Only)**

Bragg-Brentano:  Polarization Fraction:  Sample Thickness:  mm

Debye Scherrer

**Profile**

U:  V:  W:  A:  B:

Significance Limit:

**Range**

Step Width:  ° (To properly simulate synchrotron data, this value should be 0.005 or less.)

Start 2θ

Longest Line Minus:  °

Fixed Value:  °

Stop 2θ

Shortest Line Plus:  °

Fixed Value:  °

OK Cancel Apply Reset Page Reset All

*New Simulated Profile Preferences form*

## Modulated Structures

The PDF Card now supports modulated structures, which are structures that are described using more than just three-dimensional space. The new fields include:

- Additional Miller indices (h, k, l) with modulated dimensions
  - Modulated vector descriptions
    - Symmetry operators\*
    - Atomic coordinates\*

PDF Card - Bi0.06 Sr3.655 Ca1.911 Cu9.623 O16.435 - 00-061-1424

File Edit d-Spacings Tools Window Help

Wavelength: Cu Kα1 1.54056Å

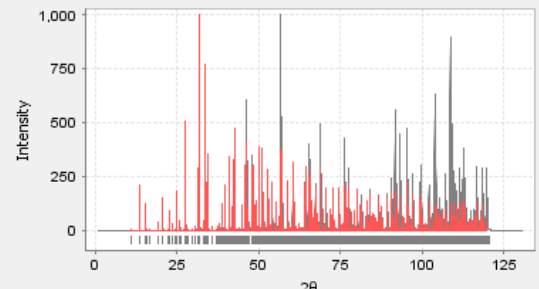
Stick Patterns:
 

- Fixed Slit Intensity
- Variable Slit Intensity
- Integrated Intensity

Diffraction Patterns:
 

- Simulated Profile
- Raw Diffraction Data (PD3)

2θ	d(Å)	I	h	k	l	M1	*
10.9117	8.10149	3	1	1	2	-3	
13.6526	6.48056	209	0	2	0	0	
15.5596	5.69034	126	2	0	0	0	
16.6736	5.31259	4	1	1	1	-2	
19.1535	4.62996	36	0	0	2	-2	
20.7565	4.27588	148	2	2	0	0	
22.2704	3.98851	5	1	3	2	-3	
22.8894	3.88203	91	2	2	1	-1	
23.5964	3.76729	29	0	2	2	-2	
24.6843	3.60366	3	3	1	2	-3	
24.7704	3.59134	6	2	0	2	-2	



00-061-1424 (Fixed Slit Intensity) — 00-061-1424 (Calculated)

PDF Experimental Physical Crystal Optical Structure Miscellaneous References Comments

TDP Type: U Origin: Crystal (Symmetry Allowed): Centrosymmetric

SG Symmetry Operators (32)

Seq	S1	S2	S3	S4	S5	S6
1	x1	x2	x3	x4		
2	-x1	x2	x3+1/2	x4		
3	x1	-x2	x3	x4+1/2		
4	-x1	-x2	-x3	-x4		
5	-x1	-x2	x3+1/2	x4+1/2		
6	x1	-x2	-x3+1/2	-x4		
7	-x1	x2	-x3	-x4+1/2		
8	x1	x2	-x3+1/2	-x4+1/2		
9	x1	x2+1/2	x3+1/2	x4+1/2		
10	-x1	x2+1/2	x3	x4+1/2		

Atomic Coordinates (7)

Fourier coefficients describing the modulation of the coordinates can be found in the CIF.

Atom	Num	x	y	z	SOF	IDP
Cu	1	0.25	0.5	0.25	1	0.0162(4)
Ca	2	0	0.38007(8)	0.25	0.321(13)	0.0081(3)

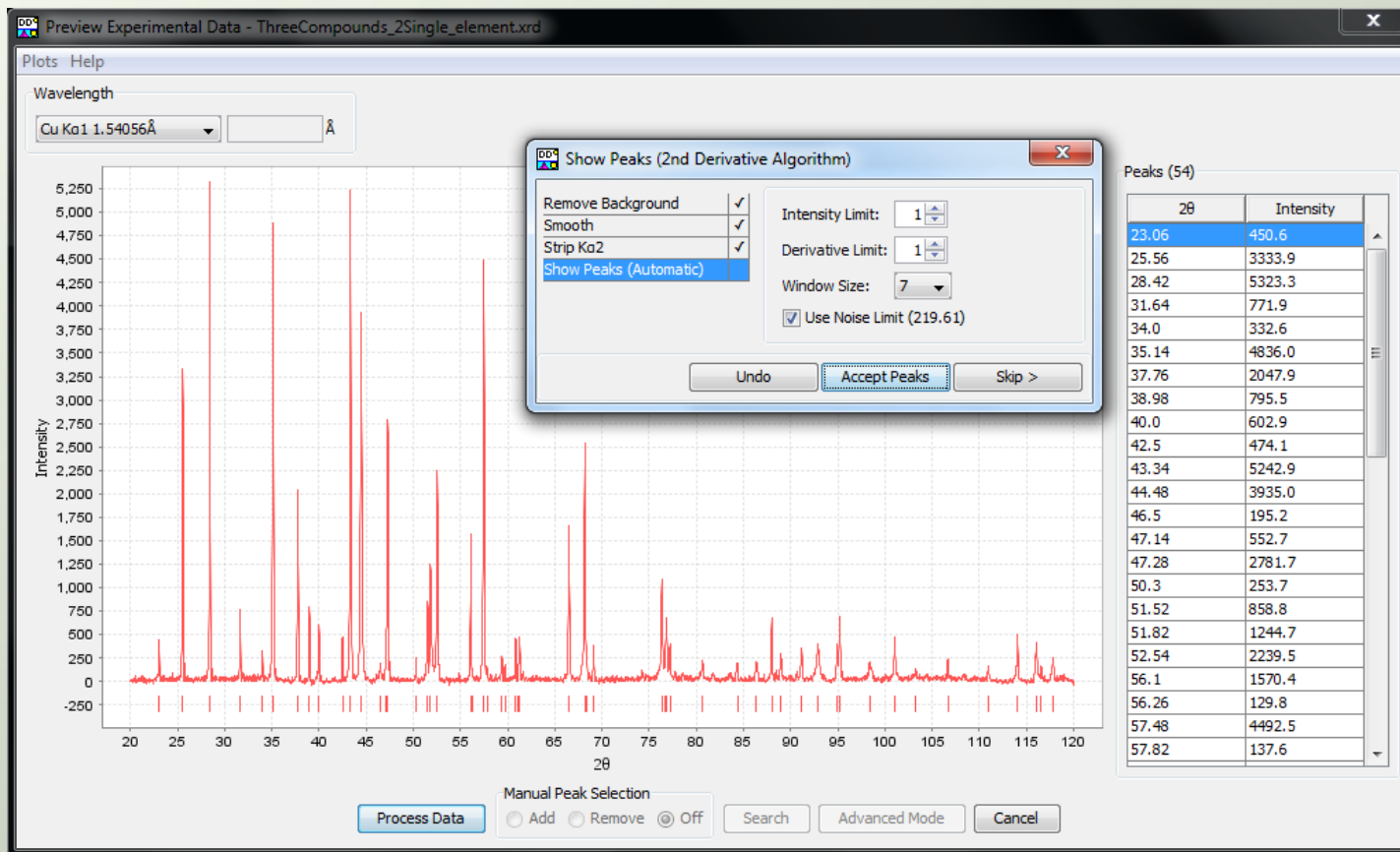
Anisotropic Thermal Displacement Parameters (7)

Atom	Num	ADP11	ADP22	ADP33	ADP12	ADP13	ADP23
Cu	1	0.01054(4)	0.0154(5)	0.0277(9)	0	0	0
Ca	2	0.0185(5)	0.0188(5)	0.0171(7)	0	0	0
Sr	3	0.0185(5)	0.0188(5)	0.0171(7)	0	0	0

## Process Experimental Data Wizard

The processing of experimental data into Sleve+ has been streamlined with a new wizard interface. This wizard interface will logically walk the user through the following processes:

- Removing the background (automatic or manual)
  - Smoothing the data
  - Stripping the  $K\alpha_2$  peaks
- Finding the peaks (automatic or manual)



Process Experimental Data Wizard showing the peak search

## Phases Summation Plot\*

Sieve+ now allows the user to view a simulation of multiple phases as a single, summed plot. This summation plot will better help the user in visually matching their experimental data to the summation of currently found phases.

Sieve+ - ThreeCompounds\_2Single\_element.xml

File Edit Matches Phases Lines Help

Matches (3,092 of 316,291)

GOM	PDF #	QM	Status	Coords	Compound Name	Chemical Formula	D1	D2	D3	D4	D5
5317	01-072-5709	I	P	✓	Calcium Magnesium Nickel	(Ca <sub>0.5</sub> Mg <sub>0.5</sub> )Ni <sub>2</sub>	2.125650	2.035160	4.070320	1.356770	1.246280
5317	04-001-4603	I	P	✓	Calcium Magnesium Nickel	Ca <sub>0.5</sub> Mg <sub>0.5</sub> Ni <sub>2</sub>	2.125650	2.035160	4.070320	1.356770	1.246280
5018	01-071-4654	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-001-1136	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-001-3177	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-002-1348	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-002-3695	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690

Matches Filter Filter Description

Select...

Experiment

Search Line(s): 2.03516 Å D1 Range: 2.029 - 2.042 Å Rotation: All

Preferences

Search Method: Hanawalt Wavelength: Cu Kα1 1.54056 Å

Search Window: 0.15 ° Match Window: 0.15 °

Lowest Allowable GOM: 2000  Weight d-Spacings

Phases (3)

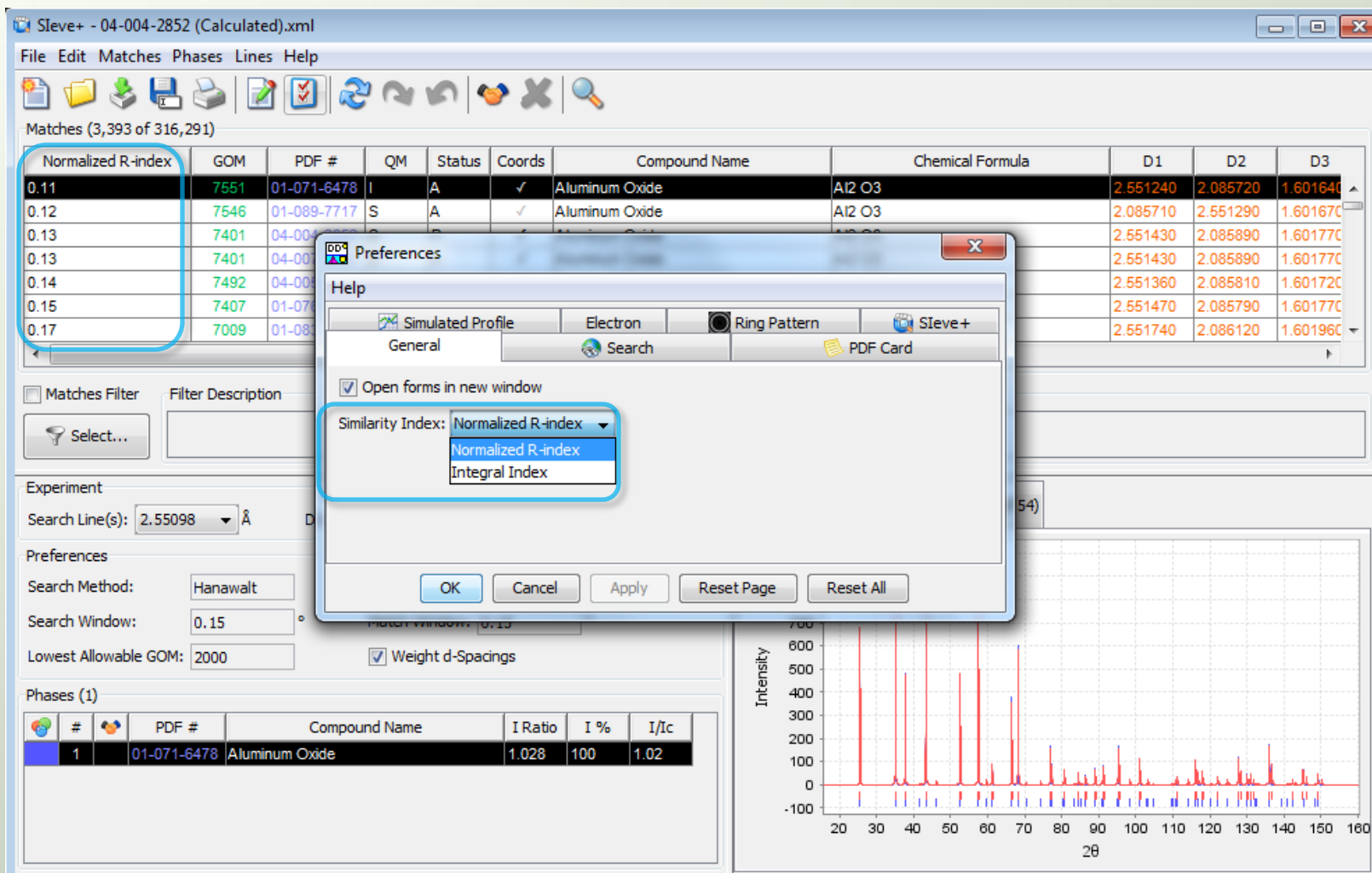
#	PDF #	Compound Name	I Ratio	I %	I/Ic
1	01-083-2080	Aluminum Oxide	0.926	35	1.0
2	04-015-2689	Silicon	1.017	38	4.56
3	01-071-4654	Nickel	0.719	27	7.44

Diffraction Patterns Lines (38 of 54)

Sieve+ form showing the summation plot (in black) at the lower right-hand side

## New Similarity Index - “Normalized R-index”\*

A new similarity index, called the “Normalized R-index”, has been developed for increased accuracy of full-pattern matching. This “Normalized R-index” is based on the R-index (Karfunkel et al. [1]) and has been modified by Dr. John Faber for use in Release 2011.



The screenshot displays the Sieve+ software interface. The main window shows a list of matches with columns for Normalized R-index, GOM, PDF #, QM, Status, Coords, Compound Name, Chemical Formula, D1, D2, and D3. A preferences dialog box is open, showing the 'Similarity Index' dropdown menu set to 'Normalized R-index'. The background shows a diffraction pattern plot with Intensity on the y-axis and 2θ on the x-axis.

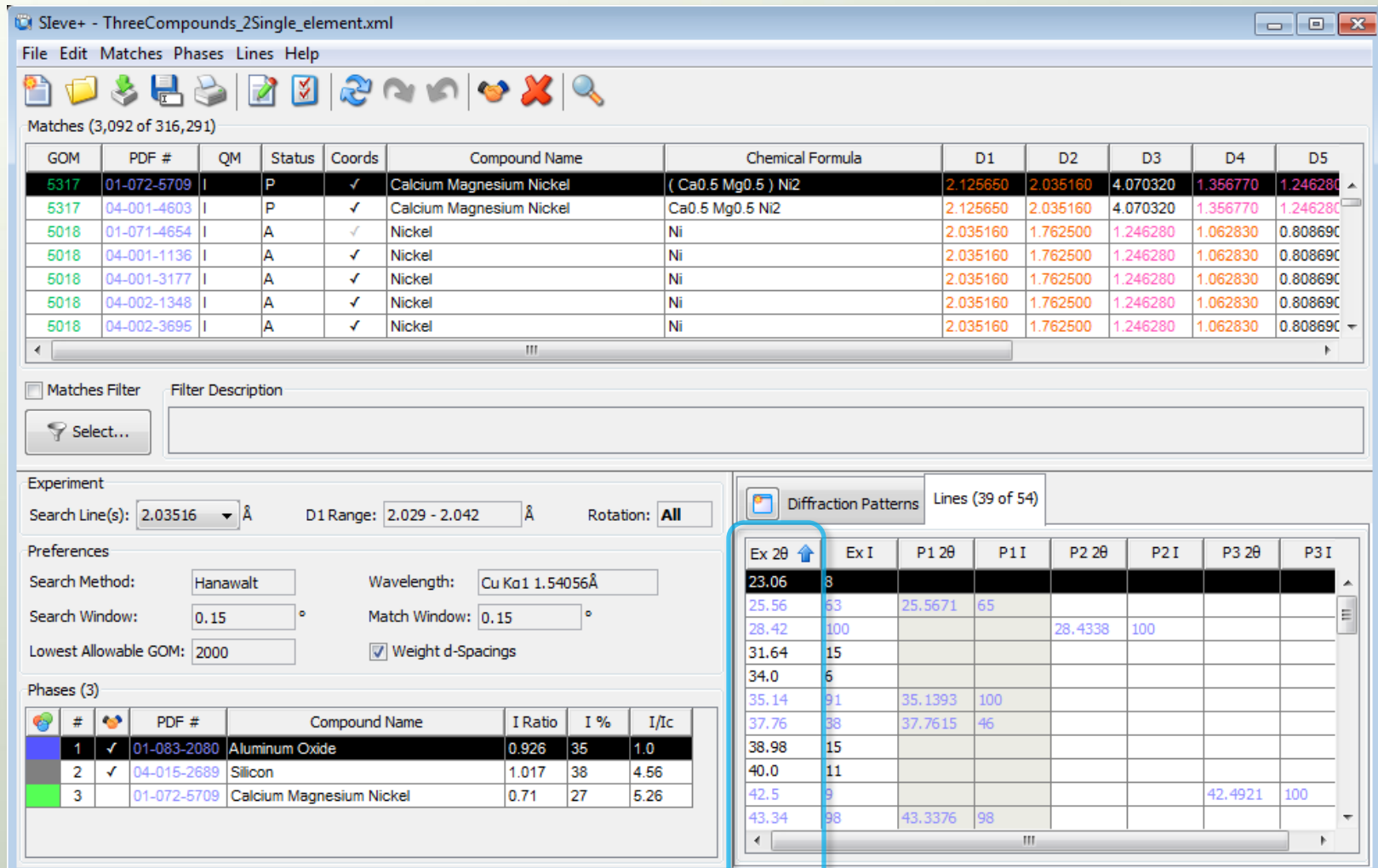
Normalized R-index	GOM	PDF #	QM	Status	Coords	Compound Name	Chemical Formula	D1	D2	D3
0.11	7551	01-071-6478	I	A	✓	Aluminum Oxide	Al <sub>2</sub> O <sub>3</sub>	2.551240	2.085720	1.601640
0.12	7546	01-089-7717	S	A	✓	Aluminum Oxide	Al <sub>2</sub> O <sub>3</sub>	2.085710	2.551290	1.601670
0.13	7401	04-004-1000						2.551430	2.085890	1.601770
0.13	7401	04-004-1000						2.551430	2.085890	1.601770
0.14	7492	04-004-1000						2.551360	2.085810	1.601720
0.15	7407	01-071-6478						2.551470	2.085790	1.601770
0.17	7009	01-089-7717						2.551740	2.086120	1.601960

#	PDF #	Compound Name	I Ratio	I %	I/Ic
1	01-071-6478	Aluminum Oxide	1.028	100	1.02

[1] Karfunkel, H.R., Rohde, B., Leusen, F.J.J., Gganitz, R.J. & Rihs, G. (1993). *J. Comput. Chem.* **14**, 1125.

# Flexible Lines Table

The Sleve+ Lines table now has the option of showing either the  $2\theta$  values (new) or the d-Spacing values.



The screenshot shows the Sleve+ software interface with the 'Lines' table displayed. The table has columns for GOM, PDF #, QM, Status, Coords, Compound Name, Chemical Formula, and d-spacings (D1-D5). Below the main table is a 'Matches Filter' section and an 'Experiment' section with search parameters. The 'Phases (3)' section lists Aluminum Oxide, Silicon, and Calcium Magnesium Nickel. The 'Diffraction Patterns' section shows a table with columns for Ex 2θ, Ex I, P1 2θ, P1 I, P2 2θ, P2 I, P3 2θ, and P3 I. The 'Ex 2θ' column is highlighted in blue, indicating that the table is showing 2θ values instead of d-spacings.

GOM	PDF #	QM	Status	Coords	Compound Name	Chemical Formula	D1	D2	D3	D4	D5
5317	01-072-5709	I	P	✓	Calcium Magnesium Nickel	(Ca <sub>0.5</sub> Mg <sub>0.5</sub> )Ni <sub>2</sub>	2.125650	2.035160	4.070320	1.356770	1.246280
5317	04-001-4603	I	P	✓	Calcium Magnesium Nickel	Ca <sub>0.5</sub> Mg <sub>0.5</sub> Ni <sub>2</sub>	2.125650	2.035160	4.070320	1.356770	1.246280
5018	01-071-4654	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-001-1136	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-001-3177	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-002-1348	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690
5018	04-002-3695	I	A	✓	Nickel	Ni	2.035160	1.762500	1.246280	1.062830	0.808690

Ex 2θ	Ex I	P1 2θ	P1 I	P2 2θ	P2 I	P3 2θ	P3 I
23.06	8						
25.56	63	25.5671	65				
28.42	100			28.4338	100		
31.64	15						
34.0	6						
35.14	91	35.1393	100				
37.76	38	37.7615	46				
38.98	15						
40.0	11						
42.5	9					42.4921	100
43.34	98	43.3376	98				

Sleve+ form showing the  $2\theta$  values in the Lines table



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

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Fax: 610.325.9823