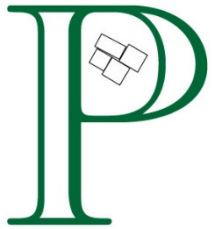
An Introduction to ICDD and the Powder Diffraction File

James A. Kaduk

Poly Crystallography, Inc., Naperville IL 60540

kaduk@polycrystallography.com



NORTH CENTRAL COLLEGE 1861

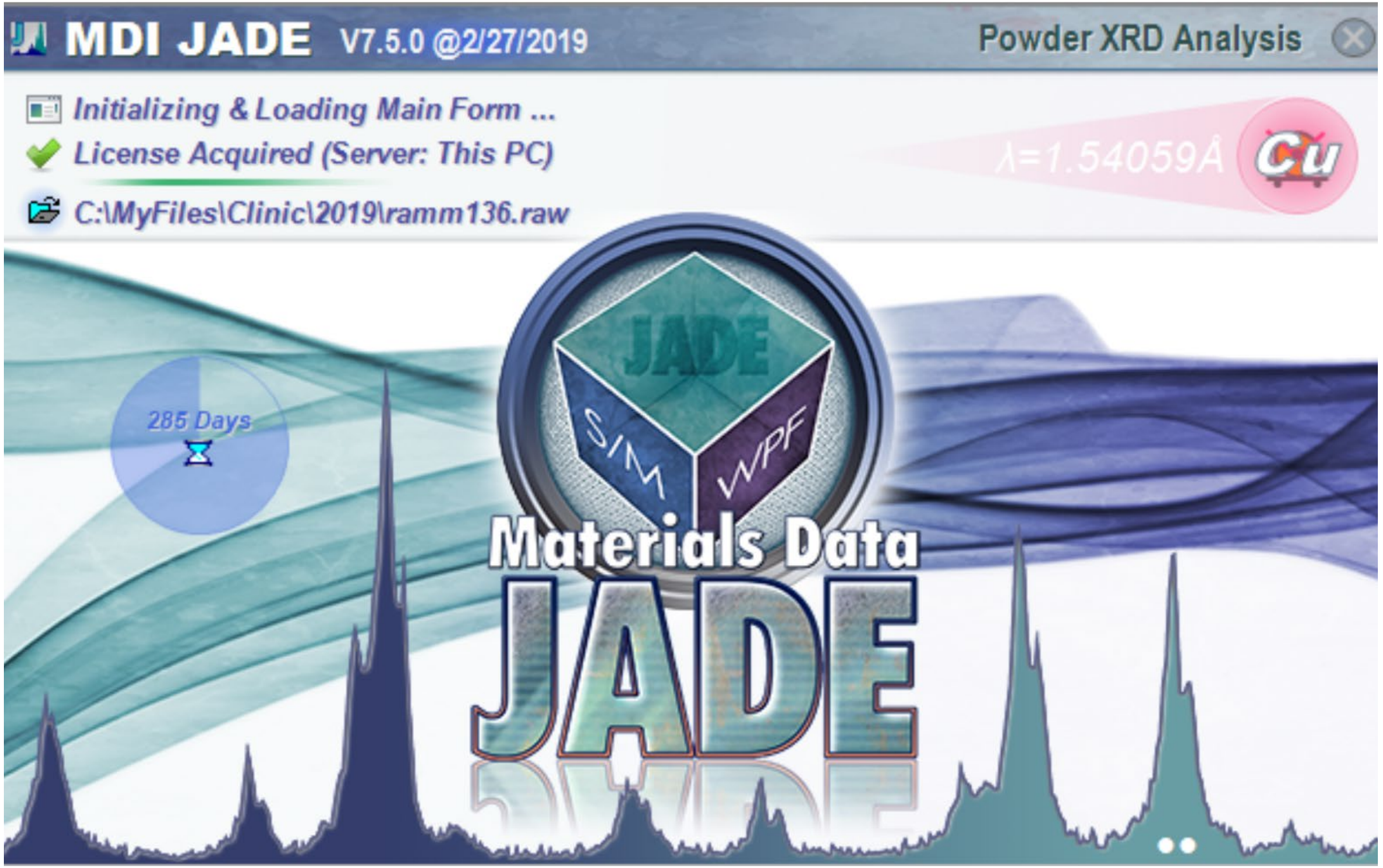
ILLINOIS INSTITUTE OF TECHNOLOGY

History

- Hanawalt, J. D. & Rinn, H. W. (1936). *Identification of crystalline materials. Ind. Eng. Chem. Anal. Ed.* **8**, 244-247, reprinted in (1986) *Powder Diffraction* **1**, 2-6.
- Hanawalt, J. D., Rinn, H. W. & Frevel, L. K. (1938). *Chemical analysis by X-ray diffraction. Ind. Eng. Chem. Anal. Ed.* **10**, 457-512, reprinted in part in (1986) *Powder Diffraction* **1**, 7-14.
- 1941 - Joint Committee for Chemical Analysis by Powder Diffraction Methods, supported by Committee E-4 of the American Society for Testing and Materials (ASTM)
- 1969 - independent non-profit Joint Committee on Powder Diffraction Standards (JCPDS).
- 1978 - name change to the International Centre for Diffraction Data

Products and Services

- PDF-2 (5 year) – 316,820 entries (2021)
- PDF-4+ (annual) – 444,133 (2021)
- PDF-4 Organics – 547,295 (2021)
- WebPDF-4, PDF-4 Minerals (48,946), PDF-4/Axiom (97,789)
- SIeve/SIeve+
- *Powder Diffraction, Advances in X-ray Analysis*
- Denver X-ray Conference, Pharmaceutical Powder Diffraction Symposium
- Clinics and Workshops
- Grant-in-Aid


MDI JADE V7.5.0 @2/27/2019
Powder XRD Analysis
Initializing & Loading Main Form ...
License Acquired (Server: This PC)
λ=1.54059Å
Cu
C:\MyFiles\Clinic\2019\ramm136.raw
285 Days
JADE
SIM
WPF
Materials Data
JADE

PDF-4+ 2019

File Edit Window Help

Open PDF Cards | Preferences | Search | History | Results | SIeve+ | Microanalysis

Search

Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
  - No Subclass
  - Depressant
  - Narcotic
  - Pesticide & Antimicrobial
  - Psychotropic
  - Stimulant

Environment
- [ ] Ambient
- [ ] Non-ambient
  - [ ] Temp.
  - [ ] Press.
  - [ ] Temp. & Press.

Status
- [x] Primary
- [x] Alternate
- [ ] Deleted

Quality Mark
- Star
- Good
- Indexed
- Calculated
- Prototyping
- Minimal Acceptable
- Blank
- Low-Precision
- Hypothetical

Database
- [ ] ICDD (00)
- [ ] ICSD (01)
- [ ] CSD (02)
- [ ] NIST (03)
- [ ] LPF (04)
- [ ] ICDD Crystal Data (05)

- [ ] Atomic Coordinates
- [ ] Raw Diffraction Data

Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

(◉) Boolean ( ) Yes/No/Maybe ( ) Composition Diagram List

(◉) And ( ) Or [ ] Not Grouping: (◉) And ( ) Or

[ ] Only ( ) Just

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.811	6 C 12.01	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
3	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.065	17 Cl 35.453	18 Ar 39.948
4	19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.941	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.993	28 Ni 58.693	29 Cu 63.546	30 Zn 65.409	31 Ga 69.723	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.798
5	37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	43 Tc [98]	44 Ru 101.07	45 Rh 102.906	46 Pd 106.42	47 Ag 107.868	48 Cd 112.41	49 In 114.818	50 Sn 118.71	51 Sb 121.76	52 Te 127.6	53 I 126.904	54 Xe 131.293
6	55 Cs 132.905	56 Ba 137.327		72 Hf 178.49	73 Ta 180.948	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.967	80 Hg 200.59	81 Tl 204.383	82 Pb 207.2	83 Bi 208.98	84 Po [209]	85 At [210]	86 Rn [222]
7	87 Fr [223]	88 Ra [226]		104 Rf [261]	105 Db [262]	106 Sg [266]	107 Bh [264]	108 Hs [277]	109 Mt [268]	110 Ds [271]	111 Rg [272]	112 Cn [285]	113 Nh [286]	114 Fl [289]	115 Mc [289]	116 Lv [293]	117 Ts [294]	118 Og [294]
La			57 La 138.906	58 Ce 140.116	59 Pr 140.908	60 Nd 144.242	61 Pm [145]	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.925	66 Dy 162.5	67 Ho 164.93	68 Er 167.259	69 Tm 168.934	70 Yb 173.04	71 Lu 174.967	
Ac			89 Ac [227]	90 Th 232.038	91 Pa 231.036	92 U 238.029	93 Np [237]	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 [262]	

Search | Reset Tab | Reset All | Help | Range Input ▼ | Global Operator ▼

Search

$Ag_{0.8}Cu_{0.2}Bi_3S_5$?

Ag, Cu, Bi, S only

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Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
  - No Subclass
  - Depressant
  - Narcotic
  - Pesticide & Antimicrobial
  - Psychotropic
  - Stimulant

Environment
- [ ] Ambient
- [ ] Non-ambient
  - [ ] Temp.
  - [ ] Press.
  - [ ] Temp. & Press.

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- [x] Alternate
- [ ] Deleted

- [ ] Atomic Coordinates
- [ ] Raw Diffraction Data

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- [ ] ICDD Crystal Data (05)

Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments

Formula ▼
Any Formula ...

Name ▼
Any Name ...

IMA No.
...

CAS Number
...

Number of Elements
Low High

Composition ▼
Element Weight % ± Error

Search | Reset Tab | Reset All | Help | Range Input ▼ | Global Operator ▼

[Only (Cu And Ag And Bi And S)] And [Status (Primary, Alternate)]

Search

Herbertsmithite

Name + Ambient + Coordinates

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Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

Mineral Classification ▼
- AEN - Aenigmatite (group)
- ALC - Allactite (group)
- VRL - Alluaudite (group)
- ALM - Alum (group)
- ALN - Alunite (supergroup)
- AMB - Amblygonite (group)
- AMP - Amphibole (family)
- ANC - Analcime (supergroup)
- ANY - Ancylite (supergroup)
- ADA - Andalusite (group)
- ANT - Antlerite (group)
- APA - Apatite (group)
- APH - Aphthitalite (supergroup)
- APO - Apophyllite (supergroup)
- ARA - Aragonite (group)
- ARC - Arcanite (group)

Zeolite Classification ▼
- ABW - Li-A(BW)
- ACO - ACP-1
- AEI - AlPO4-18
- AEL - AlPO4-11
- AEN - AlPO-EN3
- AET - AlPO4-8
- AFG - Afghanite
- AFI - AlPO4-5
- AFN - AlPO-14
- AFO - AlPO4-41
- AFR - SAPO-40
- AFS - MAPSO-46
- AFT - AlPO4-52
- AFX - SAPO-56
- AFY - CoAPO-50
- AHT - AlPO4-H2

Organic Functional Group ▼
- >4_Hetero_atoms_in_ring(s)
- >5_fused_rings
- >9_membered_ring
- 1_Hetero_atom_in_ring(s)
- 1,2_dione____O=C-C=O
- 2_fused_rings
- 2_Hetero_atoms_in_ring(s)
- 3_fused_rings
- 3_Hetero_atoms_in_ring(s)
- 3_membered_ring
- 4_fused_rings
- 4_Hetero_atoms_in_ring(s)
- 4_membered_ring
- 5_fused_rings
- 5_membered_ring
- 6_membered_ring

Pearson Symbol ▼
With Hydrogen ...

Prototype Structure ▼
Any Prototype Structure ...

Formula Type (ANX) ▼
...

Search | Reset Tab | Reset All | Help | Range Input ▼ | Global Operator ▼

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Zeolite MFI

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Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
  - No Subclass
  - Depressant
  - Narcotic
  - Pesticide & Antimicrobial
  - Psychotropic
  - Stimulant

Environment
- [ ] Ambient
- [ ] Non-ambient
  - [ ] Temp.
  - [ ] Press.
  - [ ] Temp. & Press.

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- [x] Alternate
- [ ] Deleted

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- [ ] ICDD Crystal Data (05)

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Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

Crystal System
- [ ] Triclinic (Anorthic)
- [ ] Monoclinic
- [ ] Orthorhombic
- [ ] Tetragonal
- [ ] Rhombohedral
- [ ] Hexagonal
- [ ] Cubic

Crystal (Symmetry Allowed) ▼
- [ ] Centrosymmetric
- [ ] Non-centrosymmetric:
  - [ ] Enantiomorphic
  - [ ] Pyro / Piezo (p)
  - [ ] Optical Activity
  - [ ] Piezo (2nd Harm.)

Atomic Environment Type

Symbol	Elements
1#a	Ac
2#a	Ag
2#b	Al
3#a	Am
3#b	Ar

Space Group ▼

Space Group Number ...

Crystal Data | Reduced Cell | Author's Unit Cell | Supercell/Subcell

Axis (Å)				Axial Ratio		Volume	
a:	Value ± Error	α:	Value ± Error	c/a:	Value ± Error	Value	± Error
b:	Value ± Error	β:	Value ± Error	a/b:	Value ± Error		
c:	Value ± Error	γ:	Value ± Error	c/b:	Value ± Error		

Search | Reset Tab | Reset All | Help | Range Input ▼ | Global Operator ▼

Search

Author's Unit Cell

P-orthorhombic

$a = 9.623, b = 10.565, c = 9.219$

Change esd on volume to 10 Å^3

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  - Pesticide & Antimicrobial
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Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

Modulated Dimension

[ ] 3 + 1d [ ] 3 + 2d [ ] 3 + 3d

Subsystems

[ ] Modulated Structure (One Subsystem) [ ] Composite Structure (Multiple Subsystems)

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Na3.919 (C O3)2 - 05-001-0286

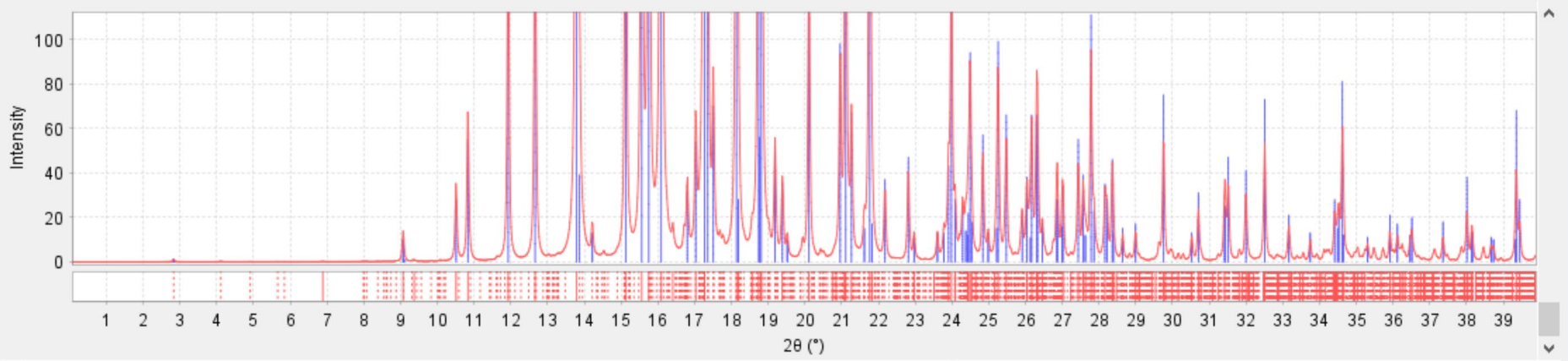
File Plots Help

Export ▼ Print | Temperature Series Toolbox Property Sheet | 2D 3D Bonds | SAED EBSD Ring | Simulated Profile Raw Diffraction Data

X-ray Diffraction
Wavelength: Custom ... Kα1: 0.709318
Neutron Diffraction
Electron Diffraction

Simulated Profile (Calc)
Raw Diffraction Data
Fixed Slit Intensity

2θ (°)	d (Å)	I	h	k	l	m	*
2.82640	14.38051	1	0	0	1	-2	
9.06742	4.48677	10	1	1	0	0	
9.08515	4.47803	1	1	1	0	-2	
10.50935	3.87255	27	-2	0	1	0	
10.83208	3.75750	55	-1	1	1	0	
11.92629	3.41384	133m	0	0	3	-4	
11.92629	3.41384	133m	1	1	1	0	
12.65959	3.21683	164	2	0	1	0	



PDF
Experimental
Physical
Crystal
Structure
Classifications
Cross-references
References
Comments

Status: Primary | Quality Mark: Star
Environment: Ambient | Temperature: 293.0 K | Pressure: -

Phase: -
Chemical Formula: $Na_{3.919}(CO_3)_2$
Structural Formula: -
Empirical Formula: $C_2Na_{3.919}O_6$
Weight %: C11.43 Na42.88 O45.69
Atomic %: C16.78 Na32.88 O50.34

Compound Name: Sodium Carbonate
Mineral Name: Natrite | IMA No: 1981-005
Alternate Name: -
CAS Number: -

Entry Date: 09/01/2014
Modification Date: 09/01/2015 | Modifications: Dx

Search | Na3.919 (C O3)2 - 05-00...

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Na3.919 (C O3)2 - 05-001-0286

Help

Unit Cell: 1 1 1

Show Atom Labels

Show Polyhedra

Maximum Combined Bonding Radius:

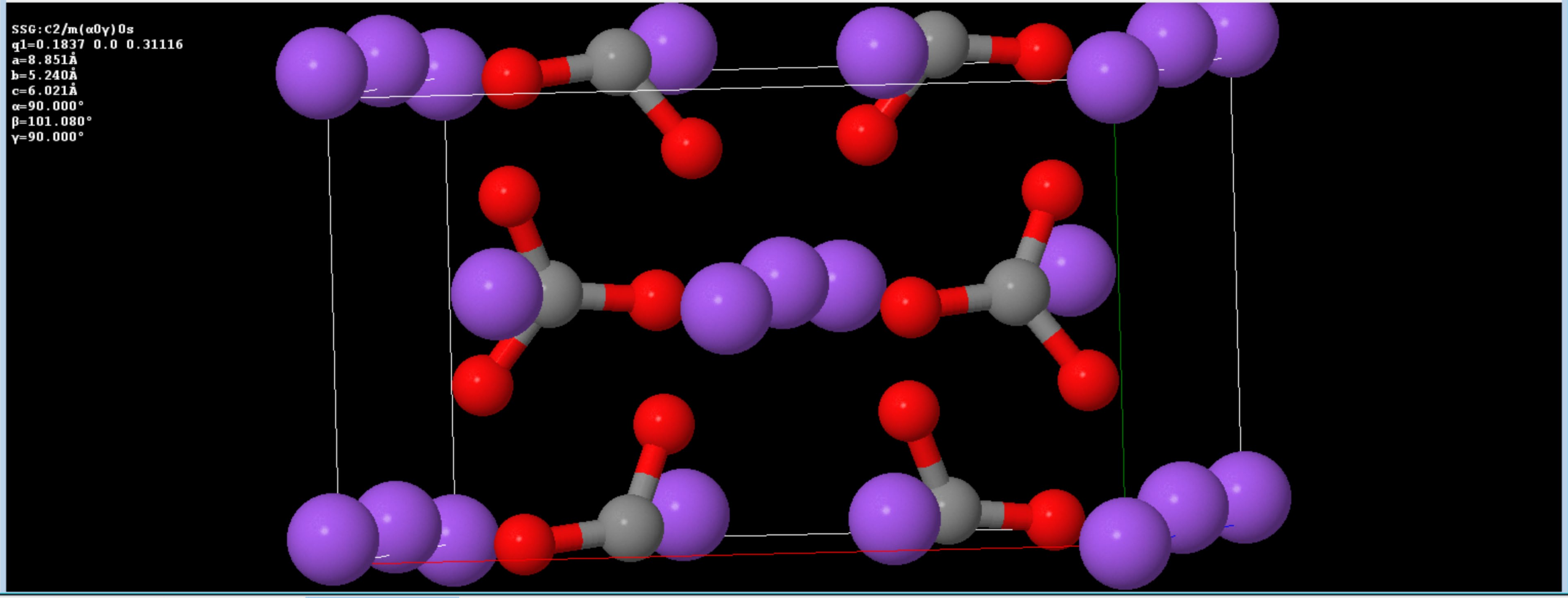
0% 25% 50% 75% 100% 125% 150%

Subsystem:

Toggle Modulation

Toggle Animation

SSG:C2/m(α0γ)0s
q1=0.1837 0.0 0.31116
a=8.851Å
b=5.240Å
c=6.021Å
α=90.000°
β=101.080°
γ=90.000°



Search | Na3.919 (C O3)2 - 05-00... | Na3.919 (C O3)2 - 05-00...

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Search

Subfile ▼

- Custom PDF Set
- Alkaloid
- Amino Acid, Peptide & Complex
- Battery Material
- Bioactive
  - No Subclass
  - Depressant
  - Narcotic
  - Pesticide & Antimicrobial
  - Psychotropic
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Environment
- [ ] Ambient
- [ ] Non-ambient
  - [ ] Temp.
  - [ ] Press.
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- [x] Primary
- [x] Alternate
- [ ] Deleted

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Database
- [ ] ICDD (00)
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- [ ] Atomic Coordinates
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Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

Radiation: (•) X-ray/Electron ( ) CW Neutron

Strong Line (Å) ▼ — Value | ± Error — [x] D1 [x] D2 [x] D3

Long Line (Å) ▼ — Value | ± Error — [x] L1 [x] L2 [x] L3

Reported Intensity — [ ] Integrated Intensities [ ] Peak Intensities

I/I-corundum ▼ — Value | ± Error

R-factor ▼ — Value | ± Error

Smith-Snyder Figure of Merit ▼ — Value | ± Error

Temperature of Data Collection (K) ▼ — Value | ± Error

Pressure of Data Collection (GPa) ▼ — Value | ± Error

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Periodic Table | Formula/Name | Classifications | Crystallography | Modulated | Diffraction | Physical Properties | Reference | Comments

Melting Point (K) ▼
Value ± Error

Density (g/cm³) ▼
Value ± Error

- [x] Measured Density
- [x] Calculated Density
- [x] Structural Density

Color ▼
- Black
- Blue
- Brown
- Color Missing
- Colorless
- Gray
- Green
- Metallic
- Orange
- Pink
- Red
- Violet
- White

- [ ] Property Sheet
- [ ] Topology Data

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(•) Search All References ( ) Search Primary Reference

DOI [...]

Title ▼ [...]

Author ▼ [...]

Publication ▼ [Journal/Patent] [...]

Volume ▼ [...]

Year [Start Year] [End Year]

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Search

Search your own surname

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Database Comments ▼

Absolute Configuration
Additional Diffraction Lines
Additional Patterns
Analysis
ANX
Atomic Position
Bioactivity
Boiling Point
Calculated Pattern Original Remarks

Search | Reset Tab | Reset All | Help | Range Input ▼ | Global Operator ▼

Search

ICSD Collection Code 88605

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Microanalysis

File Help

Element/Oxide | Weight % ▼

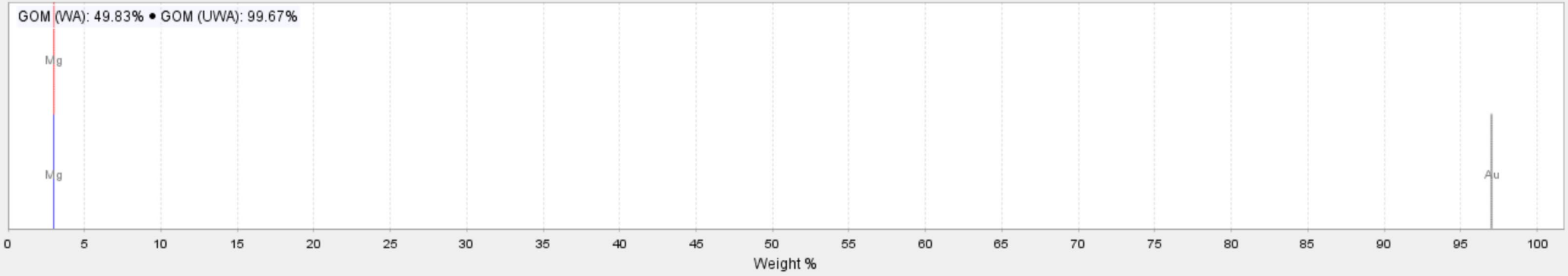
Mg | 3

± Error (%): 5.0 | Set Filter

Ignore Elements: None | [Status (Primary, Alternate)]

Matches (8,602 of 397,421)

GOM (WA)	GOM (UWA)	PDF #	QM	Weight %	Compound Name	Mineral Name
49.83%	99.67%	00-019-0519	B	Au97.01 Mg2.99	Gold Magnesium	
49.83%	99.67%	04-001-3003	P	Au97.01 Mg2.99	Gold Magnesium	
49.83%	99.67%	04-004-4093	P	Au97.01 Mg2.99	Gold Magnesium	
46.88%	93.75%	00-056-1208	B	Mg3.20 W96.80	Magnesium Tungsten	
45.17%	90.33%	04-017-8497	I	Ag97.29 Mg2.71	Magnesium Silver	
42.98%	85.96%	01-074-5964	I	Mg3.49 Sn96.51	Magnesium Tin	
42.98%	85.96%	04-003-2216	I	Mg3.49 Sn96.51	Magnesium Tin	
40.00%	80.00%	03-065-6701	I	Au96.25 Mg3.75	Gold Magnesium	
39.79%	79.58%	00-020-0456	I	Au96.23 Mg3.77	Gold Magnesium	
39.79%	79.58%	04-007-2004	I	Au96.23 Mg3.77	Gold Magnesium	
39.17%	78.33%	01-071-6824	I	Cd97.65 Mg2.35	Cadmium Magnesium	
38.33%	76.67%	04-001-0474	I	In97.70 Mg2.30	Indium Magnesium	
37.97%	75.95%	00-019-0518	I	Au96.05 Mg3.95	Gold Magnesium	
37.97%	75.95%	00-024-0461	I	Au96.05 Mg3.95	Gold Magnesium	
37.97%	75.95%	01-072-5352	I	Au96.05 Mg3.95	Gold Magnesium	
37.97%	75.95%	04-007-1482	B	Au96.05 Mg3.95	Gold Magnesium	
37.97%	75.95%	04-007-1483	B	Au96.05 Mg3.95	Gold Magnesium	
37.97%	75.95%	04-019-4954	I	Au96.05 Mg3.95	Gold Magnesium	



Search | Reset | Paste

Search | Microanalysis

Boolean Searches

Ca,Mg,C,O only and space group #167 and ambient

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Results - 10 of 412,083

File Fields Tools Help

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PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1 (Å)
00-043-0697	S	$(Ca, Mg)CO_3$	Calcium Magnesium Carbonate	Calcite, magnesian	3.004200	1.889150	2.262510	R	R-3c	4.943	16.852	356.53	3.8204
00-060-0473	I	$(Ca, Mg)(CO_3)$	Calcium Magnesium Carbonate		3.008920	1.860030	2.267010	R	R-3c	4.955	16.898	359.24	3.8240
01-086-2336	S	$(Mg_{0.129}Ca_{0.871})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian	2.999470	2.259940	1.853450	R	R-3c	4.938	16.832	355.47	3.8126
01-089-1304	S	$(Mg_{0.03}Ca_{0.97})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian, syn	3.025470	1.869360	1.904940	R	R-3c	4.978	16.988	364.57	3.8442
01-089-1305	S	$(Mg_{0.06}Ca_{0.94})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian, syn	3.018190	1.864700	1.901030	R	R-3c	4.963	16.957	361.72	3.8336
04-008-8067	B	$Ca_{0.9}Mg_{0.1}(CO_3)$	Calcium Magnesium Carbonate	Calcite, magnesian	3.002300	1.890090	1.855100	R	R-3c	4.941	16.854	356.34	3.8153
04-012-6929	S	$Ca_{0.845}Mg_{0.155}(CO_3)$	Calcium Magnesium Carbonate		3.025480	1.869370	2.278600	R	R-3c	4.978	16.988	364.57	3.8442
04-012-6930	S	$Ca_{0.715}Mg_{0.285}(CO_3)$	Calcium Magnesium Carbonate		3.018190	2.272170	1.864700	R	R-3c	4.963	16.957	361.72	3.8336
04-013-2116	S	$Ca_{0.936}Mg_{0.064}(CO_3)$	Calcium Magnesium Carbonate	Calcite, magnesian	3.020030	1.865910	1.901900	R	R-3c	4.967	16.963	362.47	3.8365
04-019-9173	P	$Ca_{0.758}Mg_{0.242}(CO_3)$	Calcium Magnesium Carbonate		2.965820	2.238700	1.833360	R	R-3c	4.896	16.600	344.60	3.7759

[Environment (Ambient)] And [Only (Mg And Ca And C And O)] And [Space Group Number Is 167] And [Status (Primary, Alternate)]

Search | Results - 10 of 412,083

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Results - 7* of 412,083 - 3 entries removed by user

File Fields Tools Help

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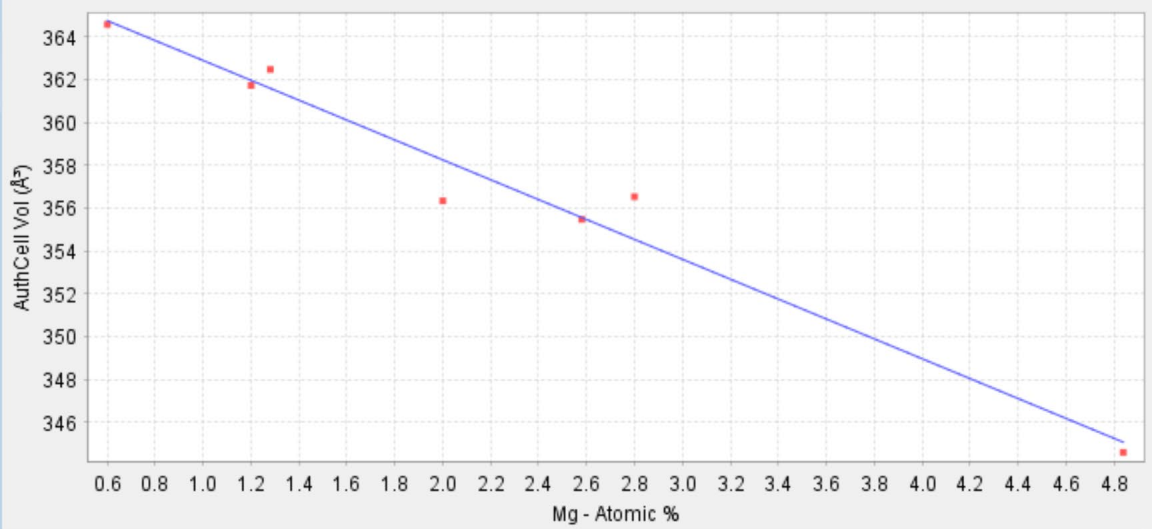
PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1 (Å)
00-043-0697	S	$(Ca, Mg)CO_3$	Calcium Magnesium Carbonate	Calcite, magnesian	3.004200	1.889150	2.262510	R	R-3c	4.943	16.852	356.53	3.8204
01-086-2336	S	$(Mg_{0.129}Ca_{0.871})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian	2.999470	2.259940	1.853450	R	R-3c	4.938	16.832	355.47	3.8126
01-089-1304	S	$(Mg_{0.03}Ca_{0.97})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian, syn	3.025470	1.869360	1.904940	R	R-3c	4.978	16.988	364.57	3.8442
01-089-1305	S	$(Mg_{0.06}Ca_{0.94})(CO_3)$	Magnesium Calcium Carbonate	Calcite, magnesian, syn	3.018190	1.864700	1.901030	R	R-3c	4.963	16.957	361.72	3.8336
04-008-8067	B	$Ca_{0.9}Mg_{0.1}(CO_3)$	Calcium Magnesium Carbonate	Calcite, magnesian	3.002300	1.890090	1.855100	R	R-3c	4.941	16.854	356.34	3.8153
04-013-2116	S	$Ca_{0.936}Mg_{0.064}(CO_3)$	Calcium Magnesium Carbonate	Calcite, magnesian	3.020030	1.865910	1.901900	R	R-3c	4.967	16.963	362.47	3.8365
04-019-9173	P	$Ca_{0.758}Mg_{0.242}(CO_3)$	Calcium Magnesium Carbonate		2.965820	2.238700	1.833360	R	R-3c	4.896	16.600	344.60	3.7759

Graphed Fields

File



[Environment (Ambient)] And [Only (Mg And Ca And C And O)] And [Space Group Number Is 167] And [Status (Primary, Alternate)]

Search | Results - 10 of 412,083 | Graphed Fields

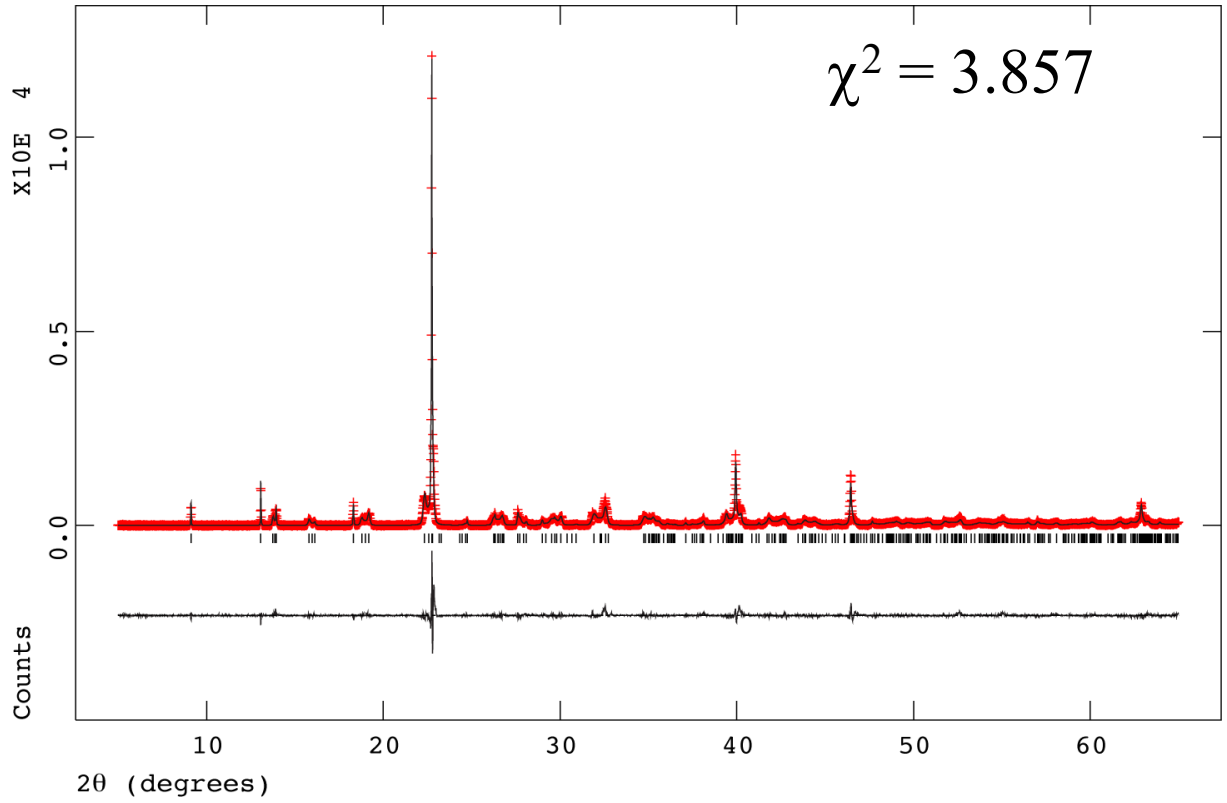
A Case Study: The 6H Perovskite $Ba_3CaSb_2O_9$

Chris Ling

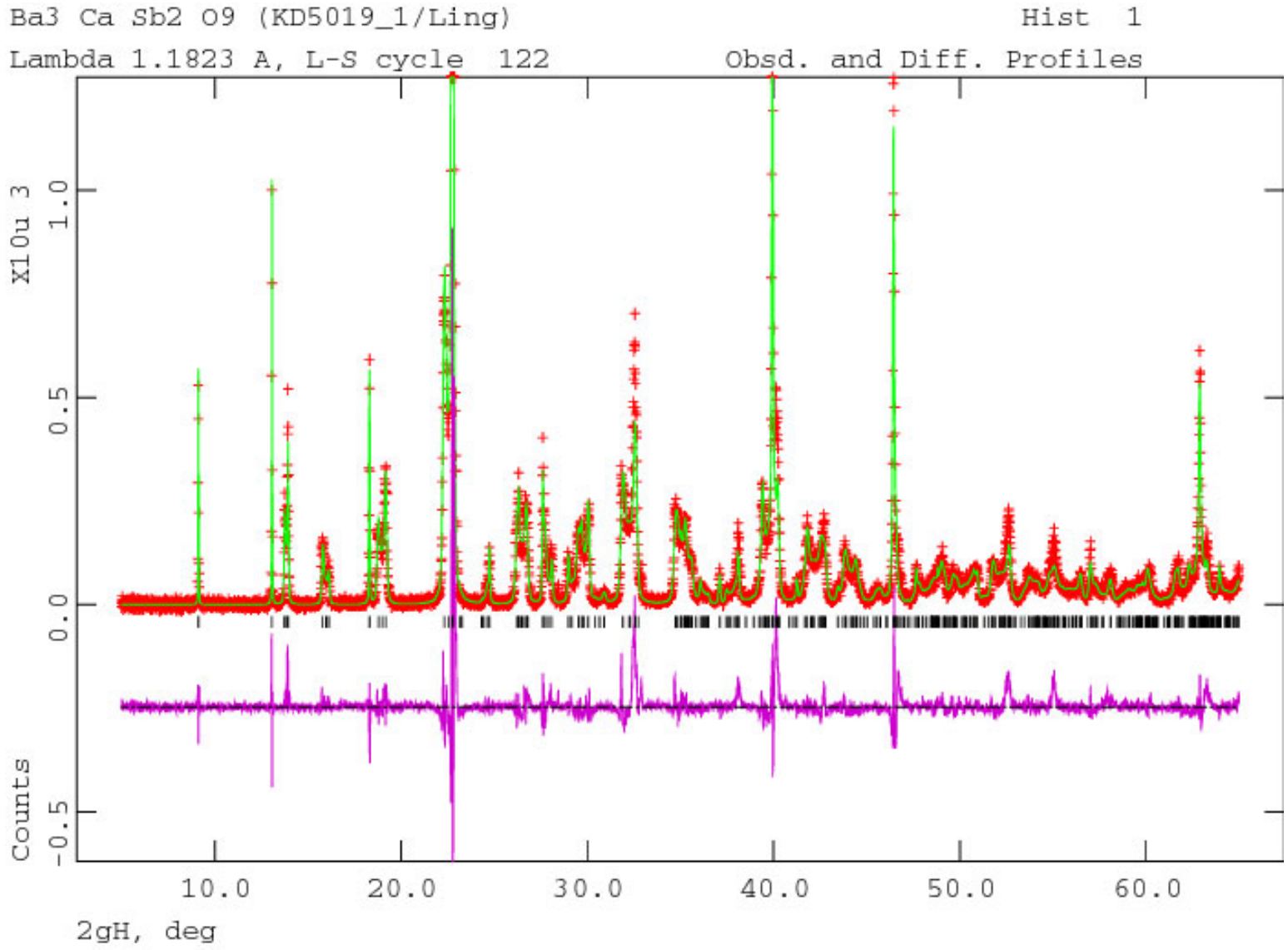
The University of Sydney

Data from 1-BM-C

C2/c, $a = 5.99898(7)$, $b = 10.37797(19)$, $c = 14.8658(3)$ Å,
$\beta = 91.384(2)°$, $V = 925.23(3)$ Å^3



Look more closely:



There are peaks unaccounted for:

2θ	d (λ = 1.182279 Å)	Intensity
22.87	2.9817	400
28.05	2.4392	70
28.44	2.4065	60
31.63	2.1619	150
32.51	2.1118	300
40.14	1.7226	260
46.70	1.4915	140
52.58	1.3346	110
55.04	1.2794	80

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Sleve+ - (Untitled)

File Help

Radiation: X-ray (0.7093187 Å)

Import 1D Diffraction Pattern
Import 2D Diffraction Pattern
New d-I List
File

Accept Phase
Remove Last Phase
Complete Phases
Action

Search Method: Hanawalt
Search Window (°): 0.3
Match Window (°): 0.3
Weight d-Spacings
2nd Pass Filter
Min GOM: 2000
Matches (3,165 of 397,421)

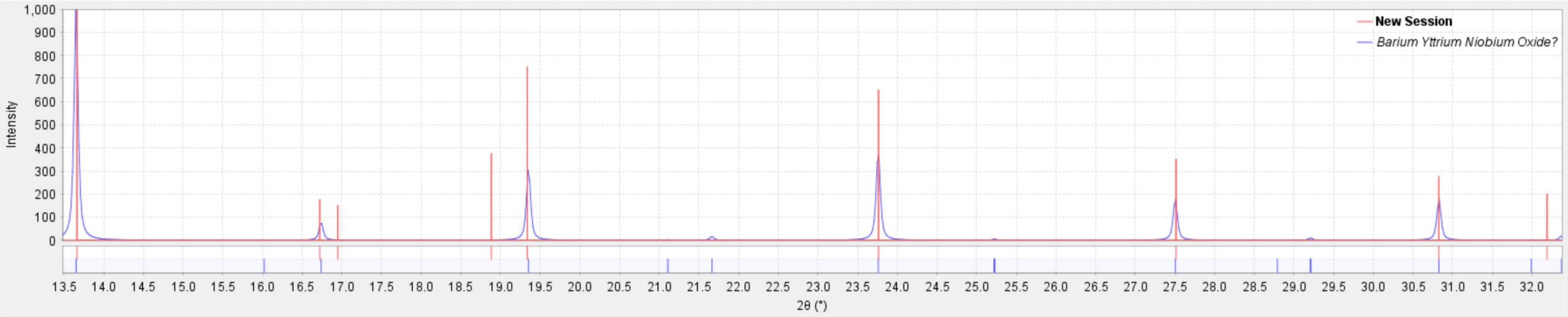
Set Filter
[Status (Primary, Alternate)]

Insert PDF
Create Graph
Table

Internal Standard
Intensity Ratios
Corrections

GOM	PDF #	Peaks Matched	Chemical Formula	Compound Name	Mineral Name	Phase	Status	QM	Coords	I/Ic	D1 (Å)	D2 (Å)	D3 (Å)	D4 (Å)	D5 (Å)
7214	04-012-0403	8 of 43 (19%)	$Ba_2 Cu_{0.10} Pr Ru_{0.90} O_6$	Barium Copper Praseodymium Ruthenium Oxide			P	I	✓	5.91	2.981660	2.108900	1.724360	2.113470	1.490830
7158	04-012-0402	8 of 50 (16%)	$Ba_2 Pr Ru O_6$	Barium Praseodymium Ruthenium Oxide			A	I	✓	5.98	2.981660	2.989740	2.108930	1.724400	2.113490
7012	01-084-9262	8 of 29 (28%)	$(Ba_{1.60} Ca_{0.40}) La Nb O_6$	Barium Calcium Lanthanum Niobium Oxide			P	I		5.38	2.980870	2.989250	2.108190	1.724000	2.113320
6870	04-022-2891	8 of 25 (32%)	$Ba_{1.6} Ca_{0.4} La Eu_x Nb O_6$	Barium Calcium Europium Lanthanum Niobium Oxide			P	P	✓	5.15	2.980890	2.989270	2.108190	1.724360	2.113340
6768	04-002-4363	7 of 14 (50%)	$Ba_2 Y Nb O_6$	Barium Yttrium Niobium Oxide			A	P	✓	15.39	2.983990	1.722810	2.110000	1.492000	1.334480
6768	04-002-6579	7 of 14 (50%)	$Ba_2 Y Zr O_6$	Barium Yttrium Zirconium Oxide			P	P	✓	15.19	2.983990	1.722810	2.110000	1.492000	1.334480
6754	04-021-7855	7 of 14 (50%)	$Ba_2 Ca_{0.79} Y_{0.13} Nb_{1.08} O_{5.68}$	Barium Calcium Yttrium Niobium Oxide			P	I	✓	14.1	2.982860	1.722150	2.109200	1.491430	1.333980
6720	04-005-7520	7 of 14 (50%)	$Ba_2 Y Nb O_6$	Barium Yttrium Niobium Oxide			A	P	✓	15.39	2.982580	1.721990	2.109000	1.491290	1.333850
6720	04-007-0162	7 of 14 (50%)	$Ba_2 Y Nb O_6$	Barium Yttrium Niobium Oxide			A	P	✓	15.39	2.982580	1.721990	2.109000	1.491290	1.333850
6705	04-015-2511	7 of 9 (78%)	$Ba Y_{0.2} Zr_{0.8} O_{2.9}$	Barium Yttrium Zirconium Oxide			P	I	✓	14.98	2.984400	1.723040	2.110290	1.492200	1.334660

Diffraction Patterns | Phases | Peaks (7 of 9)



Search | SIeve+ - (Untitled)

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Sleve+ - (Untitled)

File Help

Radiation: X-ray (0.7093187 Å)

Import 1D Diffraction Pattern
Import 2D Diffraction Pattern
New d-I List
File

Accept Phase
Remove Last Phase
Complete Phases
Action

Search Method: Fink
Search Window (°): 0.3
Match Window (°): 0.3
Weight d-Spacings
2nd Pass Filter
Min GOM: 2000
Matches (1,919 of 397,421)

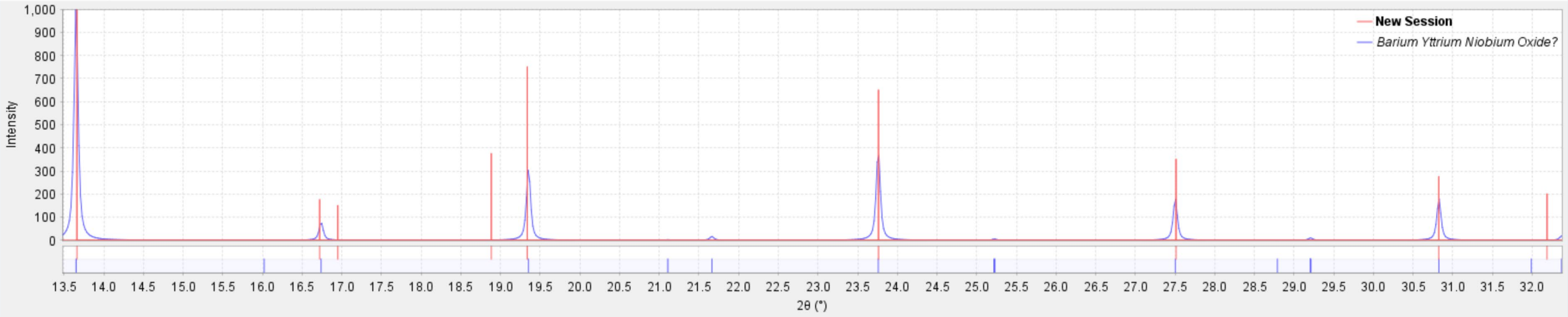
Set Filter
[Status (Primary, Alternate)]

Insert PDF
Create Graph
Table

Internal Standard
Intensity Ratios
Corrections

GOM	PDF #	Peaks Matched	Chemical Formula	Compound Name	Mineral Name	Phase	Status	QM	Coords	I/Ic	LS1 (Å)	LS2 (Å)	LS3 (Å)	LS4 (Å)	LS5 (Å)
7318	04-012-0403	8 of 43 (19%)	$Ba_2 Cu_{0.10} Pr Ru_{0.90} O_6$	Barium Copper Praseodymium Ruthenium Oxide			P	I	✓	5.91	2.981660	2.113470	2.108900	1.724360	1.494850
7184	04-018-0963	7 of 24 (29%)	$Ba_2 Y Ta O_6$	Barium Yttrium Tantalum Oxide		Low tem...	A	B	✓	11.67	2.982230	2.112070	2.105450	1.722690	1.719990
6868	01-084-9262	8 of 29 (28%)	$(Ba_{1.60} Ca_{0.40}) La Nb O_6$	Barium Calcium Lanthanum Niobium Oxide			P	I		5.38	2.989250	2.980870	2.113320	2.108190	1.724000
6854	04-022-2891	8 of 25 (32%)	$Ba_{1.6} Ca_{0.4} La Eu_x Nb O_6$	Barium Calcium Europium Lanthanum Niobium Oxide			P	P	✓	5.15	2.989270	2.980890	2.113340	2.108190	1.724360
6845	04-012-0402	8 of 50 (16%)	$Ba_2 Pr Ru O_6$	Barium Praseodymium Ruthenium Oxide			A	I	✓	5.98	2.989740	2.981660	2.113490	2.108930	1.724400
6796	04-009-4989	8 of 32 (25%)	$Ba Tl_{0.6} Sb_{0.4} O_{2.9}$	Barium Thallium Antimony Oxide			P	P	✓	13.98	2.982660	2.970000	2.112750	2.105390	1.722940
6601	04-002-4363	7 of 14 (50%)	$Ba_2 Y Nb O_6$	Barium Yttrium Niobium Oxide			A	P	✓	15.39	2.983990	2.436420	2.110000	1.722810	1.492000
6601	04-002-6579	7 of 14 (50%)	$Ba_2 Y Zr O_6$	Barium Yttrium Zirconium Oxide			P	P	✓	15.19	2.983990	2.436420	2.110000	1.722810	1.492000
6601	04-006-0345	7 of 9 (78%)	$Ba Y_{0.6} Nb_{0.2} W_{0.2} O_3$	Barium Yttrium Niobium Tungsten Oxide			P	I	✓	15.96	2.983990	2.436420	2.110000	1.722810	1.492000
6595	04-014-0985	7 of 14 (50%)	$Ba_2 Y Nb O_6$	Barium Yttrium Niobium Oxide			A	I	✓	15.31	2.984380	2.436740	2.110280	1.723030	1.492190

Diffraction Patterns | Phases | Peaks (7 of 9)



Search | SIeve+ - (Untitled)

A weak peak at 28.44° (2.4065 Å)
is still unaccounted for:

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Results - 26 of 412,083

File Fields Tools Help

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PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1 (Å)
00-004-0777	I	Ca O	Calcium Oxide	Lime, syn	2.405000	1.701000	2.778000	C	Fm-3m	4.811	4.811	111.32	2.7780
00-037-1497	S	Ca O	Calcium Oxide	Lime, syn	2.405870	1.700930	2.777370	C	Fm-3m	4.811	4.811	111.33	2.7773
00-048-1467	C	Ca O	Calcium Oxide	Lime, syn	2.405060	1.700810	2.777710	C	Fm-3m	4.811	4.811	111.33	2.7777
01-070-5490	S	Ca O	Calcium Oxide	Lime, syn	2.407600	1.702430	2.780060	C	Fm-3m	4.815	4.815	111.65	2.7800
01-077-2010	I	Ca O	Calcium Oxide	Lime, syn	2.406000	1.701300	2.778210	C	Fm-3m	4.812	4.812	111.42	2.7782
01-077-9574	S	Ca O	Calcium Oxide	Lime, syn	2.405360	1.700850	2.777470	C	Fm-3m	4.811	4.811	111.33	2.7774
01-080-7710	S	Ca O	Calcium Oxide		2.408550	1.703100	2.781150	C	Fm-3m	4.817	4.817	111.78	2.7811
01-082-1690	S	Ca O	Calcium Oxide	Lime, syn	2.402450	1.698790	2.774110	C	Fm-3m	4.805	4.805	110.93	2.7741
04-002-6758	I	Ca O	Calcium Oxide	Lime, syn	2.405000	1.700590	2.777050	C	Fm-3m	4.810	4.810	111.28	2.7770
04-003-7161	I	Ca O	Calcium Oxide	Lime, syn	2.404000	1.699880	2.775900	C	Fm-3m	4.808	4.808	111.15	2.7759
04-004-5528	I	Ca O	Calcium Oxide		2.401600	1.698190	2.773130	C	Fm-3m	4.803	4.803	110.81	2.7731
04-004-8549	I	Ba_2 Sb_3	Antimony Barium		3.095000	2.414010	3.170170	M	P21/c	15.817	6.934	1475.44	10.2476
04-004-8985	I	Ca O	Calcium Oxide	Lime, syn	2.405600	1.701020	2.777750	C	Fm-3m	4.811	4.811	111.37	2.7777
04-005-4757	I	Ca O	Calcium Oxide	Lime, syn	2.401000	1.697760	2.772440	C	Fm-3m	4.802	4.802	110.73	2.7724
04-005-6351	I	Ca O	Calcium Oxide	Lime, syn	2.407500	1.702360	2.779940	C	Fm-3m	4.815	4.815	111.63	2.7799
04-005-9402	I	Ca O	Calcium Oxide	Lime, syn	2.407500	1.702360	2.779940	C	Fm-3m	4.815	4.815	111.63	2.7799
04-006-5940	H	Ca O	Calcium Oxide	Lime, syn	2.410000	1.704130	2.782830	C	Fm-3m	4.820	4.820	111.98	2.7828
04-006-5942	I	Ca O	Calcium Oxide	Lime, syn	2.406000	1.701300	2.778210	C	Fm-3m	4.812	4.812	111.42	2.7782
04-006-6519	I	Ca O	Calcium Oxide	Lime, syn	2.400000	1.697060	2.771280	C	Fm-3m	4.800	4.800	110.59	2.7712
04-006-9375	I	Ca O	Calcium Oxide	Lime, syn	2.405000	1.700590	2.777050	C	Fm-3m	4.810	4.810	111.28	2.7770
04-007-4743	I	Ca O	Calcium Oxide	Lime, syn	2.405290	1.700800	2.777400	C	Fm-3m	4.811	4.811	111.33	2.7774
04-007-8376	I	Ca O	Calcium Oxide	Lime, syn	2.405000	1.700590	2.777050	C	Fm-3m	4.810	4.810	111.28	2.7770
04-007-9734	I	Ca O	Calcium Oxide	Lime, syn	2.409500	1.703770	2.782250	C	Fm-3m	4.819	4.819	111.91	2.7822
04-010-5778	I	Ca O	Calcium Oxide	Lime, syn	2.407600	1.702430	2.780060	C	Fm-3m	4.815	4.815	111.65	2.7800
04-011-8430	I	Ca O	Calcium Oxide	Lime, syn	2.404000	1.699880	2.775900	C	Fm-3m	4.808	4.808	111.15	2.7759
04-011-9020	I	Ca O	Calcium Oxide	Lime, syn	2.404850	1.700490	2.776880	C	Fm-3m	4.810	4.810	111.26	2.7768

[Just (Ca And Ba And Sb And O)] And [Strong Line = 2.41(0.01) Å] And [Status (Primary, Alternate)]

Search | Results - 26 of 412,083

There’s still a very weak peak at 32.89°/2.0881 Å:

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Results - 10 of 412,083

File Fields Tools Help

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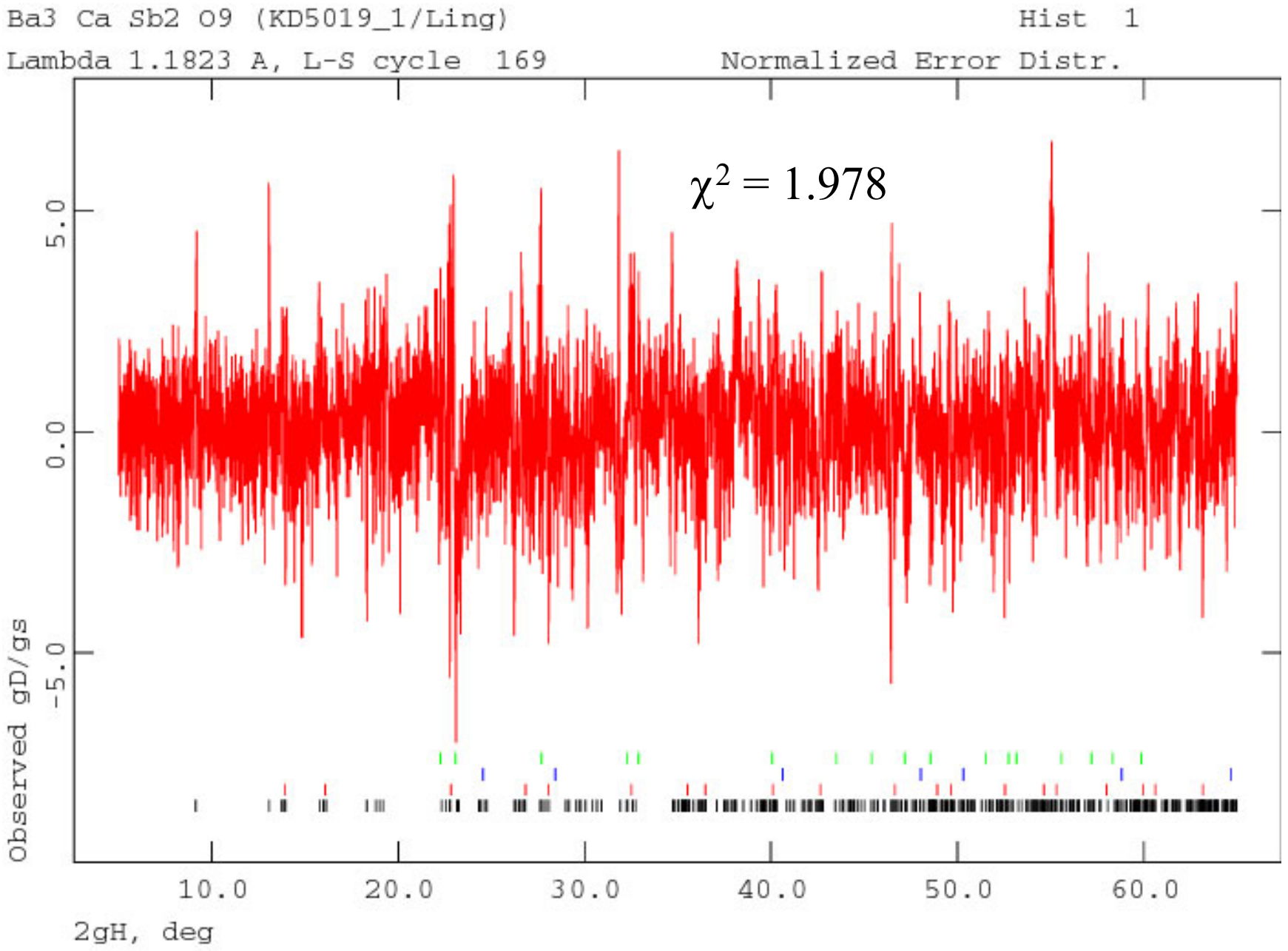
PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1 (Å)
00-017-0125	B	Sb	Antimony		2.940000	2.090000	1.710000	C	Pm-3m	2.960	2.960	25.93	2.9400
00-020-0209	O	$Ca_3 Sb_2 O_6$	Calcium Antimony Oxide		2.970000	2.880000	2.080000	X					4.4200
01-083-8080	I	O_8	Oxygen		2.158210	2.087170	3.271880	M	C2/m	6.947	3.656	139.90	4.3164
01-083-8081	S	O_8	Oxygen		2.157840	2.085380	3.275620	M	C2/m	6.963	3.657	140.01	4.3156
04-002-2786	I	Ba O	Barium Oxide		2.084070	2.899140	2.050000	T	P4/nmm	4.100	2.998	50.40	2.9980
04-007-9029	S	Sb	Antimony		2.987500	2.099000	2.126230	R	R-3m	4.198	10.485	160.02	3.4950
04-007-9030	S	Sb	Antimony		2.983760	2.098000	2.121870	R	R-3m	4.196	10.455	159.41	3.4850
04-013-2320	I	(O_2)	Oxygen		2.158210	2.087170	3.271880	M	C2/m	6.947	3.656	139.90	4.3164
04-013-2321	S	(O_2)	Oxygen		2.157840	2.085380	3.275620	M	C2/m	6.963	3.657	140.01	4.3156
04-017-1162	P	Sb	Antimony		2.929190	2.060000	2.082690	R	R-3m	4.120	10.260	150.82	3.4200

[Just (Ca And Ba And Sb And O)] And [Strong Line = 2.09(0.01) Å] And [Status (Primary, Alternate)]

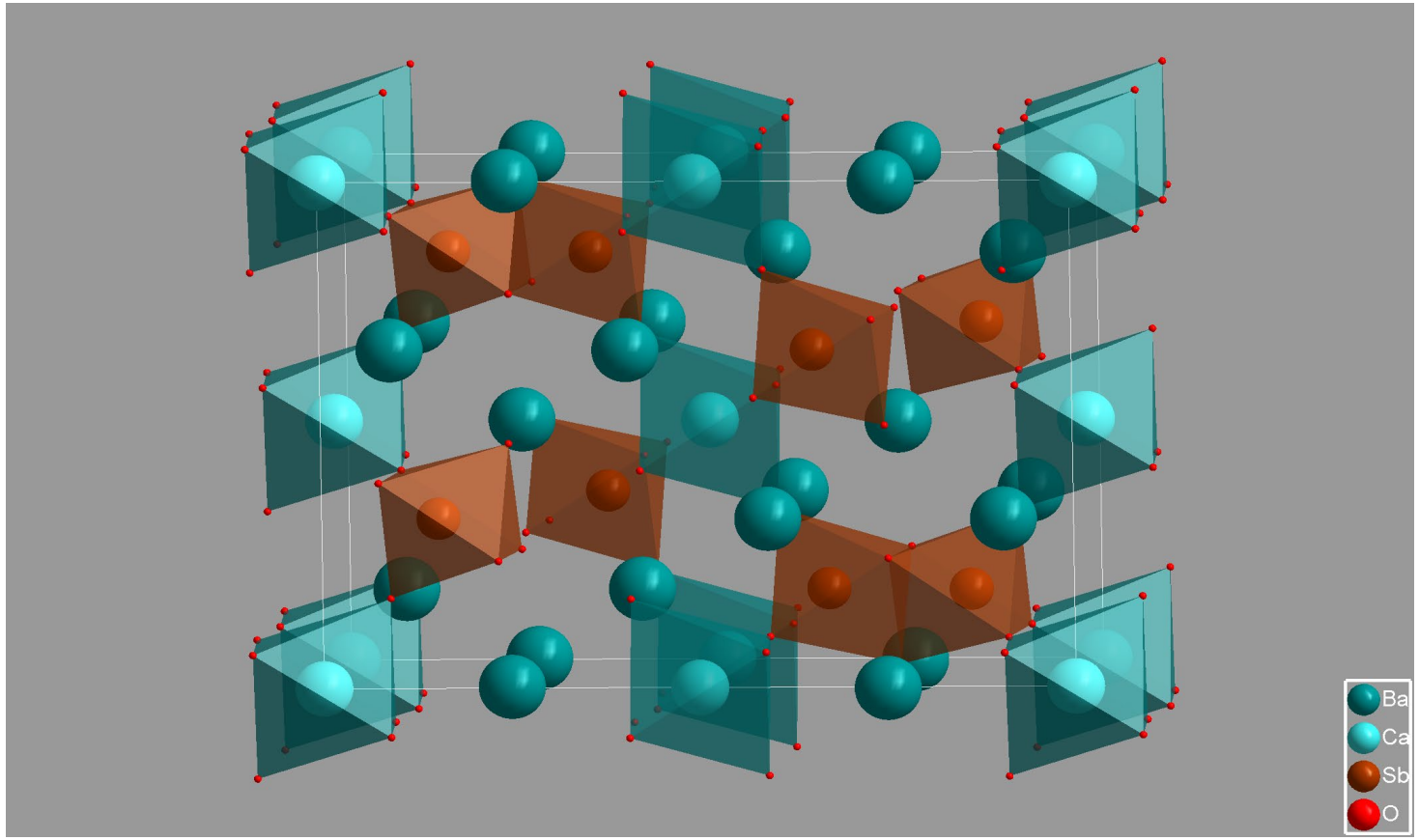
Search | Results - 10 of 412,083


Ba3 Ca Sb2 O9 (KD5019_1/Ling)
Hist 1
Lambda 1.1823 A, L-S cycle 169
Normalized Error Distr.
$\chi^2 = 1.978$
5.0
0.0
-5.0
Observed gD/gs
10.0
20.0
30.0
40.0
50.0
60.0
2gH, deg

Quantitative Phase Analysis

Phase	Concentration, wt%
$Ba_3CaSb_2O_9$	88.59(3)
Ba_2CaSbO_6	10.59(9)
CaO	0.53(3)
BaO?	0.28(2)
other	trace

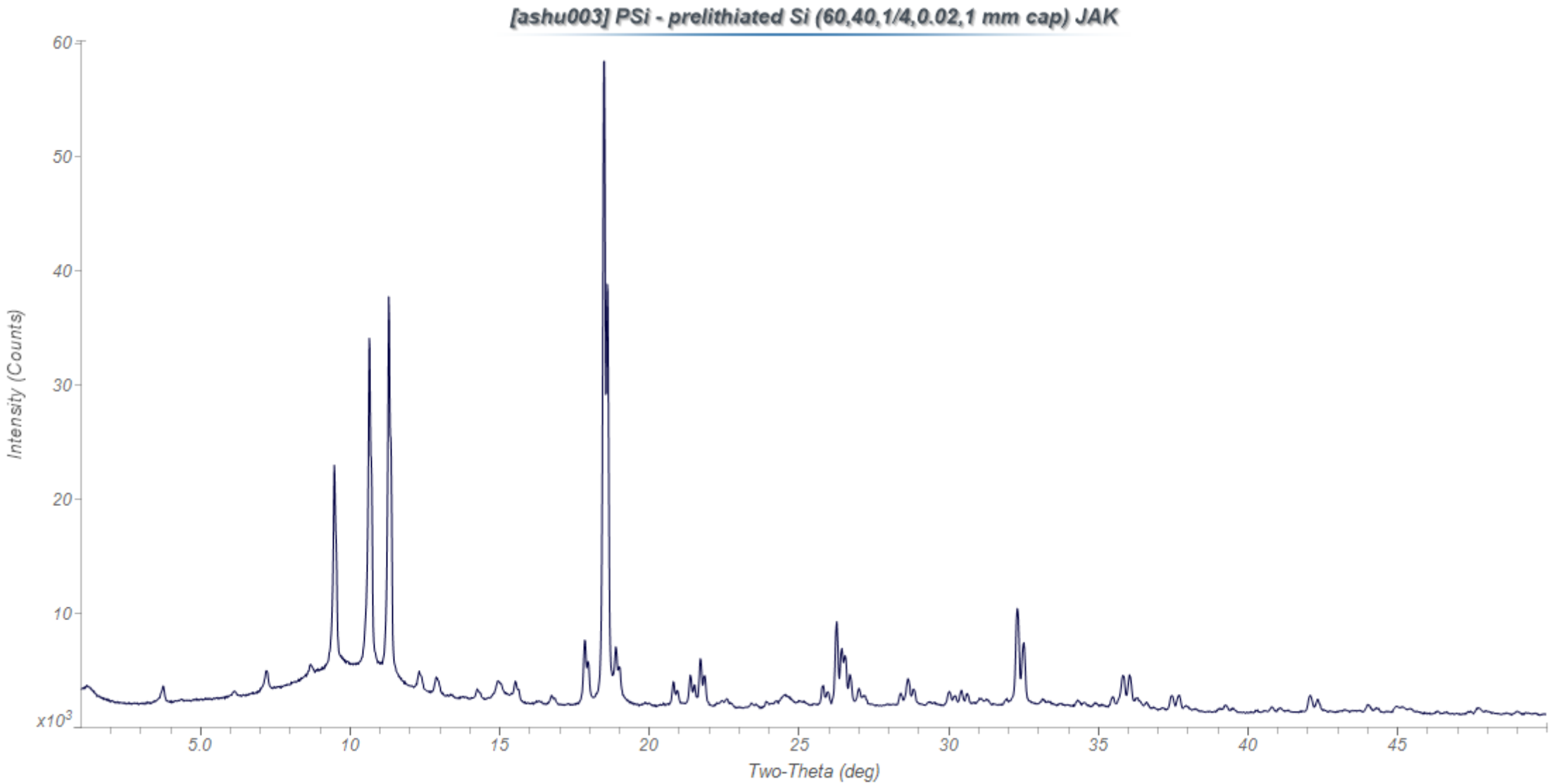
$Ba_3CaSb_2O_9$



Use of SIeve+ and JADE

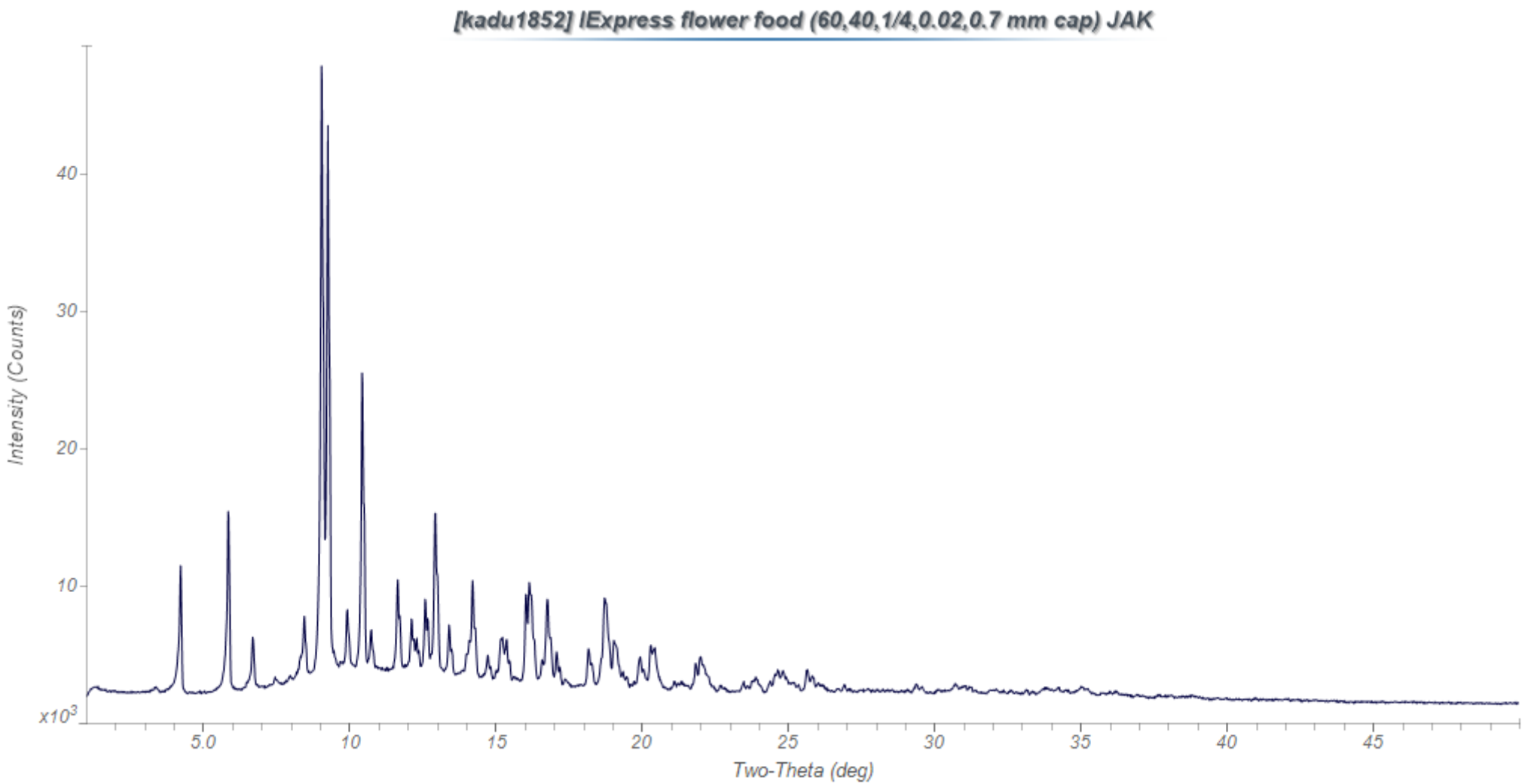
“prelithiated Si”

ashu003.xrdml


[ashu003] PSi - prelithiated Si (60,40,1/4,0.02,1 mm cap) JAK
Intensity (Counts)
x10^3
60
50
40
30
20
10
5.0
10
15
20
25
30
35
40
45
Two-Theta (deg)

IExpress flower food

kadu1852.xrdml


[kadu1852] lExpress flower food (60,40,1/4,0.02,0.7 mm cap) JAK
Intensity (Counts)
40
30
20
10
x10^3
5.0
10
15
20
25
30
35
40
45
Two-Theta (deg)

Supplied with PDF-4

“Sessions”

Inorganic Phases

- **Exercise 7-1-1.** Believed to be a pure phase, but not sure that the label on the reagent bottle is correct.
- **Exercise 7-1-2.** A student tried to prepare $SrTiO_3$ using reagent SrO, but the reaction did not go as planned. Check the SrO.
- **Exercise 7-1-3.** Check the product of a preparation of $CdTiO_3$ to see if it is phase pure.

Inorganic Phases

- **Exercise 7-1-4.** A mixture of three common oxides.
- **Exercise 7-1-5.** A smear mount of a natural specimen of witherite, $BaCO_3$.
- **Exercise 7-1-6.** A white paint.
- **Exercise 7-1-7.** A black filter deposit from a filter in a new solar hot water system. XRF indicates Fe, Ca, and minor Mg. An acid test indicates the presence of carbonate.

Inorganic Phases

- **Exercise 7-1-8.** A sample of lime (prepared by heating calcite at 1000°C) was left exposed to the air for several days. What is it now?
- **Exercise 7-1-9.** A synthetic red phosphor for color television tubes.
- **Exercise 7-1-10.** A fluorescent screen (which turns out to be a solid solution).

Minerals

- **Exercise 7-2-1.** A natural specimen of a zinc mineral. Consider data quality of old PDF entries and associations.
- **Exercise 7-2-2.** A mixture of polymorphs.
- **Exercise 7-2-3.** A mixture prepared to simulate the pressure-induced changes which can be induced by severe grinding. The specimen was prepared without any special care to avoid preferred orientation.

Minerals

- **Exercise 7-2-4.** An attempt to estimate the composition of a solid solution mineral.
- **Exercise 7-2-5.** A hydrothermal ore containing a trace of gold.
- **Exercise 7-2-6.** Typical raw material used to make dental ceramics (the best grade of whiteware porcelain). It is mined from a pegmatite deposit. We are asked to identify the feldspar(s) present.

Minerals

- **Exercise 7-2-7.** A mixture of sulfide minerals.
- **Exercise 7-2-8.** A mineral with low-angle lines and an impurity.
- **Exercise 7-2-9.** The < 2μm fraction of a sedimentary rock (sandstone).

Metals and Alloys

- **Exercise 7-3-1.** An artificial example to build confidence in identifying multi-phase unknowns
- **Exercise 7-3-2.** A steel
- **Exercise 7-3-3.** A corrosion product from a white metal bearing. XRF indicates the presence of Sn, with small amounts of Cu and Sb.

Organic Phases

- **Exercise 7-4-1.** A tablet, ground to a fine powder and smeared on a zero-background holder.
- **Exercise 7-4-2.** A potassium-containing compound isolated from a winery.
- **Exercise 7-4-3.** The product of an organic synthesis which used both NaOH and HCl.
- **Exercise 7-4-4.** A complete unknown.

Organic Phases

- **Exercise 7-4-5.** An over-the-counter medication.
- **Exercise 7-4-6.** A white powder found in an abandoned house.
- **Exercise 7-4-7.** An over-the-counter pharmaceutical.
- **Exercise 7-4-8.** A pharmaceutical which is known to contain sulfur.
- **Exercise 7-4-9.** A mixture which is known to contain CN, Cl, and COOH groups.
- **Exercise 7-4-10.** A prescription medication which is known to contain S by XRF.