Data retrieval and Structure determination
from Synchrotron Powder Diffraction data
April 3-5 2013

The Powder Diffraction Database

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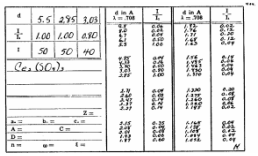
4 April 2013

INTRODUCTION



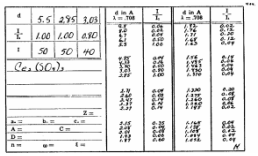
1. INTRODUCCTION

What's a powder diffraction database?
The Powder Diffraction File
Databases and search-match programs

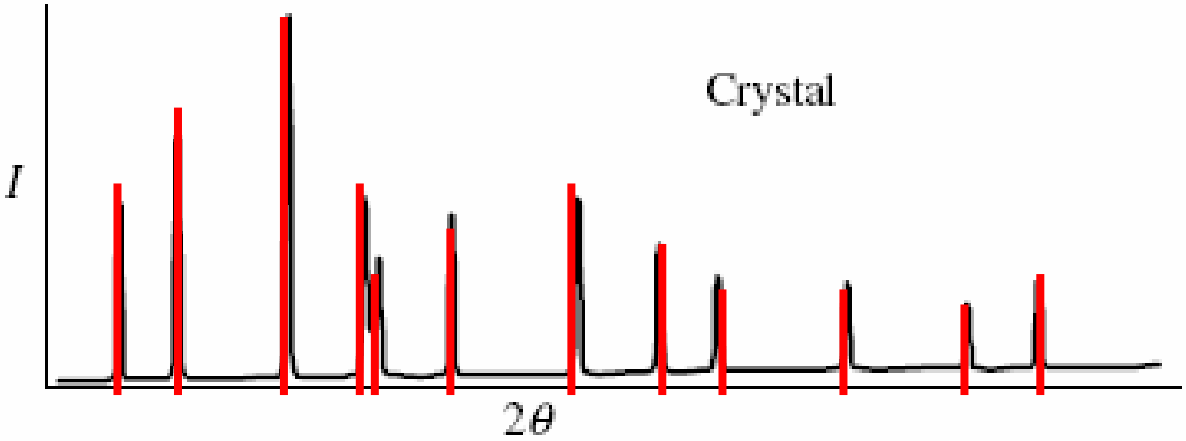
2. PDF DATABASE - ICDD

Powder Diffraction File Database
Exemples PDF-4+
- Search Filters (3)
- Sleve+ Program (1)
- Export atomic coordinates (1)

3. OTHER SPECIFIC DATABASES



Powder diffraction ⟶ IDENTIFICATION and CHARACTERIZATION



DATABASES

33-1161 ★

SiO_2

Silicon Oxide

Quartz, syn

Rad. CuKα1 λ 1.540598 Filter Mono. d-sp Diff.
Cut off Int. Diffractometer $I/I_{cor.}$ 3.6
Ref. Natl. Bur. Stand. (U.S.) Monogr. 25, 18 61 (1981)

Sys. Hexagonal S.G. $P3_221$ (154)
a 4.9133(2) b c 5.4053(4) A C 1.1001
α β γ Z 3 mp
Ref. Ibid.

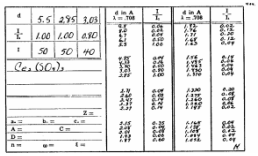
D_x 2.65 D_m 2.66 SS/FOM F_{30} =77(.013,31)

εα nωβ 1.544 εγ 1.553 Sign + 2V
Ref. Swanson, Fuyat, Natl. Bur. Stand. (U.S.), Circ. 539, 3 24 (1954)

Color Colorless
Pattern taken at 25 C. Sample from the Glass Section at NBS, Gaithersburg, Maryland, USA, ground single-crystals of optical quality. Pattern reviewed by Holzer, J., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid (1990). Agrees well with experimental and calculated patterns. O_2Si type. Quartz group. Also called: silica. Also called: low quartz. Silicon used as internal standard. PSC: hP9. To replace 5-490 and validated by calculated pattern. Plus 6 additional reflections to 0.9089.

dÅ	Int	hkℓ	dÅ	Int	hk
4.257	22	100	1.1532	1	311
3.342	100	101	1.1405	<1	204
2.457	8	110	1.1143	<1	303
2.282	8	102	1.0813	2	312
2.237	4	111	1.0635	<1	400
2.127	6	200	1.0476	1	105
1.9792	4	201	1.0438	<1	401
1.8179	14	112	1.0347	<1	214
1.8021	<1	003	1.0150	1	223
1.6719	4	202	0.9898	1	402
1.6591	2	103	0.9873	1	313
1.6082	<1	210	0.9783	<1	304
1.5418	9	211	0.9762	1	320
1.4536	1	113	0.9636	<1	205
1.4189	<1	300			
1.3820	6	212			
1.3752	7	203			
1.3718	8	301			
1.2880	2	104			
1.2558	2	302			
1.2285	1	220			
1.1999	2	213			
1.1978	1	221			
1.1843	3	114			
1.1804	3	310			

INTRODUCTION: Past and Present



1895
X-ray Röentgen

1913
Bragg's law

X-ray diffraction

1930s Dow Chemical Company scientists (Hanawalt)

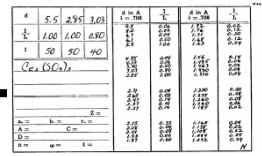
1941 The Joint Committee for Chemical Analysis by Powder Diffraction Methods

Powder Diffraction File (PDF) → *ASTM*

1969 *The Joint Committee on Powder Diffraction Standards (JCPDS)*

1978 *International* Centre for Diffraction Data

INTRODUCTION: Past and Present



Primary referei

d	5.5	2.85
$\frac{I}{I_1}$	1.00	1.10
I	50	
$Ce_2(SO_4)$		
$a_o =$	$b_o =$	
A =		
D =		
n =	ω =	

1941

00-046-1045 Sep 5, 2012 10:11 AM (jgil)

Status Primary **QM:** Star (S) **Pressure/Temperature:** Ambient **Chemical Formula:** Si O2
Empirical Formula: O2 Si **Weight %:** O53.26 Si46.74 **Atomic %:** O66.67 Si33.33
Compound Name: Silicon Oxide **Mineral Name:** Quartz, syn

Radiation: CuKα1 **λ:** 1.5406Å **Filter:** Ge Mono **d-Spacing:** Diff. **Intensity:** Diffractometer **I/Ic:** 3.41

SYS: Hexagonal **SPGR:** P3221 (154)
Author's Cell [AuthCell a: 4.91344(4)Å **AuthCell c:** 5.40524(8)Å **AuthCell Vol:** 113.01Å³ **AuthCell Z:** 3.00
AuthCell MolVol: 37.67] **Author's Cell Axial Ratio [c/a:** 1.100] **Dcalc:** 2.649g/cm³ **Dmeas:** 2.66g/cm³
SSIFOM: F(30) = 558.3(0.0017, 31)

Space Group: P3221 (154) **Molecular Weight:** 60.08
Crystal Data [XtlCell a: 4.913Å **XtlCell b:** 4.913Å **XtlCell c:** 5.405Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
XtlCell γ: 120.00° **XtlCell Vol:** 113.01Å³ **XtlCell Z:** 3.00]
Crystal Data Axial Ratio [c/a: 1.100 **a/b:** 1.000 **c/b:** 1.100]
Reduced Cell [RedCell a: 4.913Å **RedCell b:** 4.913Å **RedCell c:** 5.405Å **RedCell α:** 90.00°
RedCell β: 90.00° **RedCell γ:** 120.00° **RedCell Vol:** 113.01Å³]

πωβ: =1.544 **εγ:** =1.553 **Sign:** =+

Crystal (Symmetry Allowed): Centrosymmetric

Pearson: hP9.00 **Prototype Structure:** Si O2 **Prototype Structure (Alpha Order):** O2 Si
LPF Prototype Structure: Si O2,hP9,152 **LPF Prototype Structure (Alpha Order):** O2 Si
Mineral Classification: Quartz (Supergroup), Class Member

Subfile(s): Inorganic, Pharmaceutical (Excipient), Primary Pattern, Metals & Alloys, Mineral Related (Mineral , Synthetic), Common Phase, Forensic, Cement and Hydration Product

Entry Date: 01/24/1995 **Last Modification Date:** 01/11/2011
Cross-Ref PDF #'s: 00-033-1161 (Alternate), 01-085-0335 (Alternate), □ 04-005-4494 (Alternate), □ 04-012-0490 (Primary)

References:

Type	Reference
Primary Reference	Kern, A., Eysel, W., Mineralogisch-Petrograph. Inst., Univ. Heidelberg, Germany. ICDD Grant-in-Aid (1993).
Optical Data	Swanson, Fuyat. Natl. Bur. Stand. (U. S.), Circ. 539 3, 24 (1954).
Structure	Z. Kristallogr. 196, 177 (1992).

Database Comments: Additional Patterns: To replace 00-033-1161. See PDF 01-085-0335. Color: White. General Comments: Low temperature quartz. 2θ determination based on profile fit method. Temperature of Data Collection: Pattern taken at 296(1) K. Unit Cell Data Source: Powder Diffraction.

d-Spacings (58) - 00-046-1045 (Fixed Slit Intensity) - Cu Kα1 1.54056Å

2θ	d(Å)	I	h	k	l	*	2θ	d(Å)	I	h	k	l	*	2θ	d(Å)	I	h	k	l	*
20.8595	**4.254990**	16	1	0	0		77.6730	1.228320	1	2	2	0		114.0566	0.918159	<1	3	2	2	
26.6393	**3.343470**	100	1	0	1		79.8817	1.199820	2	2	1	3		114.4625	0.916060	2	4	0	3	
36.5431	2.456870	9	1	1	0		80.0444	1.197790	<1	2	2	1		114.6347	0.915176	2	4	1	1	
39.4641	2.281490	8	1	0	2		81.1707	1.183990	2	1	1	4		115.8806	0.908890	<1	2	2	4	
40.2989	2.236130	4	1	1	1		81.4888	1.180170	2	3	1	0		117.5323	0.900851	<1	0	0	6	
42.4490	2.127710	6	2	0	0		83.8377	1.152980	1	3	1	1		118.3081	0.897188	<1	2	1	5	
45.7918	1.979860	4	2	0	1		84.9548	1.140650	<1	2	0	4		120.1191	0.888910	1	3	1	4	
50.1375	**1.817960**	13	1	1	2		87.4366	1.114550	<1	3	0	3		121.8479	0.881352	<1	1	0	6	
50.6206	1.801740	<1	0	0	3		90.8284	1.081550	2	3	1	2		122.5998	0.878167	<1	4	1	2	
54.8734	1.671730	4	2	0	2		92.7853	1.063800	<1	4	0	0		127.2452	0.859796	<1	3	0	5	
55.3235	1.659190	2	1	0	3		94.6476	1.047720	1	1	0	5		131.1967	0.845837	<1	1	1	6	
57.2338	1.608270	<1	2	1	0		95.1154	1.043800	<1	4	0	1		132.7495	0.840746	<1	5	0	1	
59.9584	1.541530	9	2	1	1		96.2345	1.034610	1	2	1	4		134.2862	0.835918	<1	4	0	4	
64.0340	1.452890	2	1	1	3		98.7472	1.014900	1	2	2	3		136.4169	0.829560	1	2	0	6	
65.7842	1.418410	<1	3	0	0		102.2275	0.989576	<1	1	1	5		137.8875	0.825393	2	4	1	3	
67.7421	1.382100	6	2	1	2		102.5635	0.987246	<1	3	1	3		140.3102	0.818911	<1	3	3	0	
68.1420	1.374960	7	2	0	3		103.8733	0.978345	<1	3	0	4		143.2423	0.811682	3	5	0	2	
68.3161	1.371880	5	3	0	1		104.1994	0.976174	<1	3	2	0		144.1101	0.809688	<1	3	3	1	
73.4658	1.287910	2	1	0	4		106.5892	0.960785	<1	3	2	1								
75.6577	1.255950	3	3	0	2		112.1098	0.926526	<1	4	1	0								

Int	hkℓ
14	

Mar 7, 2013 1:19 PM (jgil)

Pressure/Temperature: Ambient **Chemical Formula:** Ce2 (S O4)3
t %: Ce49.30 O33.78 S16.92 **Atomic %:** Ce11.76 O70.59 S17.65

acing: D.S. **Camera Diameter:** 406.40

Dmeas: 3.912g/cm³

[XtlCell Vol: 0.00Å³]

etric

Primary Pattern, Common Phase, Educational Pattern

L. Anal. Chem. 10, 457 (1938).

en. General Comments: Color and measured density from Data on Chemicals for al Research Council Bulletin 107. Decomposition temperature is 920 C at 746 Source: Powder Diffraction.

ensity) - Cu Kα1 1.54056Å

	d(Å)	I	h	k	l	*	2θ	d(Å)	I	h	k	l	*
22	2.270000	14					65.1846	1.430000	4				
79	2.150000	35					68.4228	1.370000	4				
16	2.080000	4					71.4006	1.320000	20				
70	2.010000	8					73.9952	1.280000	8				
50	1.930000	6					75.3719	1.260000	8				
03	1.870000	60					78.3036	1.220000	6				
75	1.820000	2					80.6758	1.190000	2				
92	1.760000	12					82.3497	1.170000	4				
59	1.710000	20					85.0146	1.140000	2				
07	1.680000	12					87.8866	1.110000	2				
18	1.630000	4					89.9307	1.090000	4				
72	1.560000	14					94.3781	1.050000	4				
72	1.500000	4											
54	1.460000	4											

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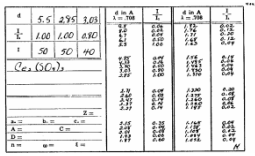

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45.7918	1.979860	4	2	0	1		84.9548	1.140650	<1	2	0	4		120.1191	0.888910	1	3	1	4	
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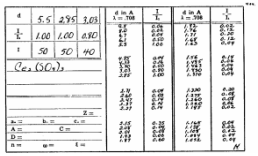
73.4658	1.287910	2	1	0	4		106.5892	0.960785	<1	3	2	1								
75.6577	1.255950	3	3	0	2		112.1098	0.928526	<1	4	1	0								

INTRODUCTION: Identification= database+search-match program

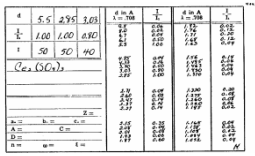


Identification of crystalline phases in powder diffraction

powder diffraction database containing reference information	+	search-match program

- ✓ICDD-Powder Diffraction File
- ✓ICSD-Inorganic Crystal Structure Data
- ✓CSD-Cambridge Structural Database
- ✓NIST-Crystal Data
- ✓Pauling's File
- ✓CRYSMET-Metals and alloys Database
- ✓PDB-Protein Data Bank
- ✓Mineralogy Database
- ✓IZA-Zeolite Database
- ✓COD- Crystallographic Open Database

- ✓Sieve -ICDD
- ✓DIFFRACplus SEARCH – Bruker AXS GmbH
- ✓X'Pert HighScore – PANalytical B. V
- ✓Crystallographica Search-Match – Oxford CrCryosytems Ltd.
- ✓Jade-Materials Data
- ✓MATCH! – Crystal Impact
- ✓MadDiff-MacDiff
- ✓AXES-H. Mändar and T. Vajakas, AXES
- ✓WinXRD – Thermo Electron Corporation



Powder Diffraction File - PDF

760,019 material data sets

- ✓Diffraction data
- ✓Crystallographic data
- ✓Bibliographic data

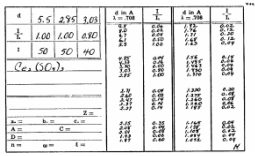
Data entry source	PDF-2 Release 2012	PDF-4+2012 WebPDF-4+ 2012	PDF-4/Minerals 2012	PDF-4/Organics 2013
Total No. of Data Sets	**250,182**	**328,660**	**39,410**	**471,257**
00- ICDD	108,711	108,711	11,548	33,727
01- FIZ	131,404	59,927	11,094	6,132
02- CCDC	0	0	0	431,359
03- NIST	10,067	3,122	208	39
04- MPDS	0	156,900	16,560	0

PDF-2
- inorganic materials
- rapid material identification

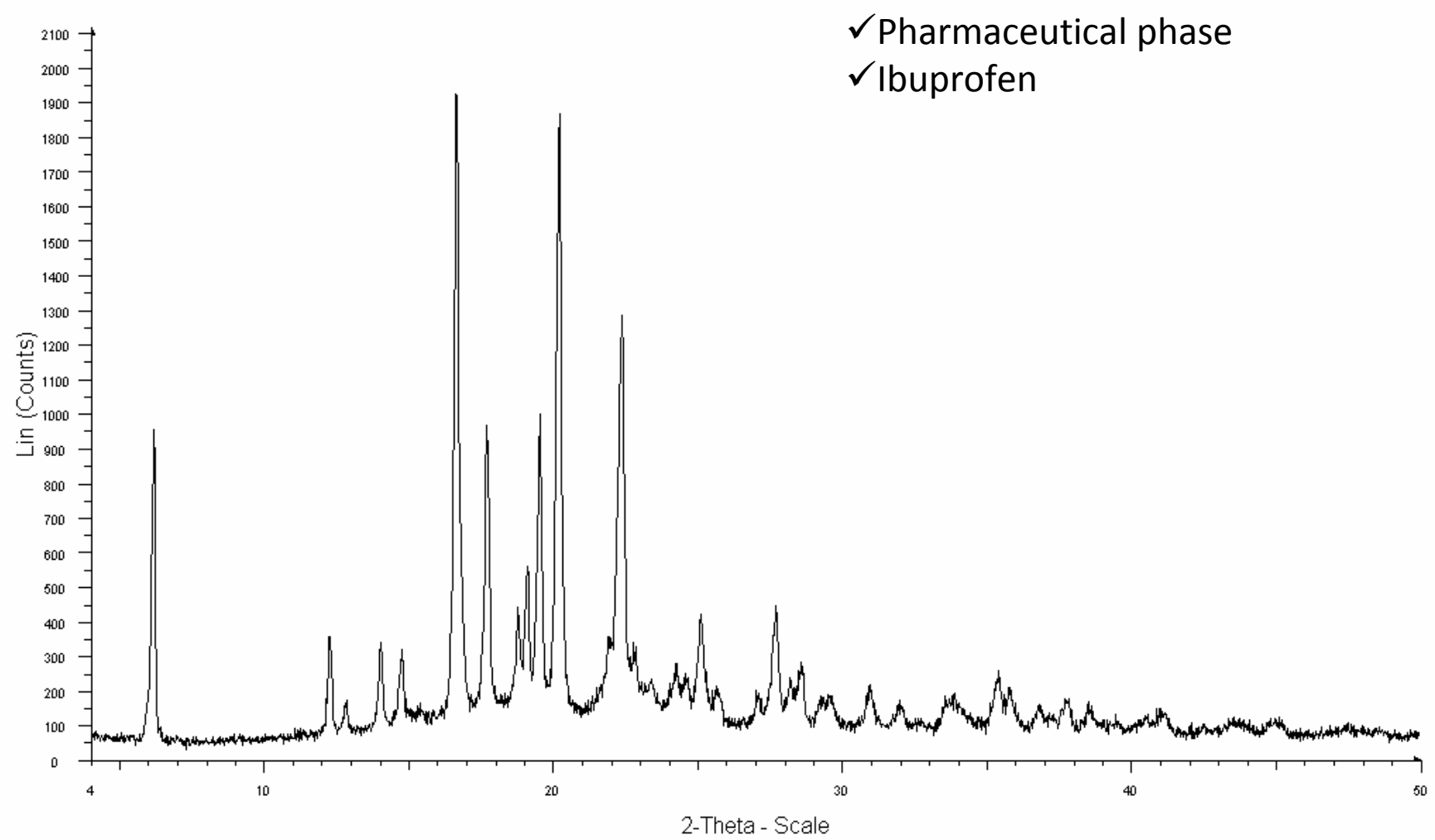
PDF-4+
- most advanced database
- identification and quantitative analysis

PDF-4 /Minerals
- 90% all know minerals

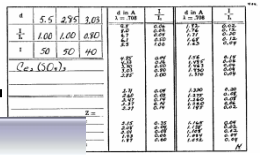
PDF-4 /Organics
- World's largest x-ray powder database for organics

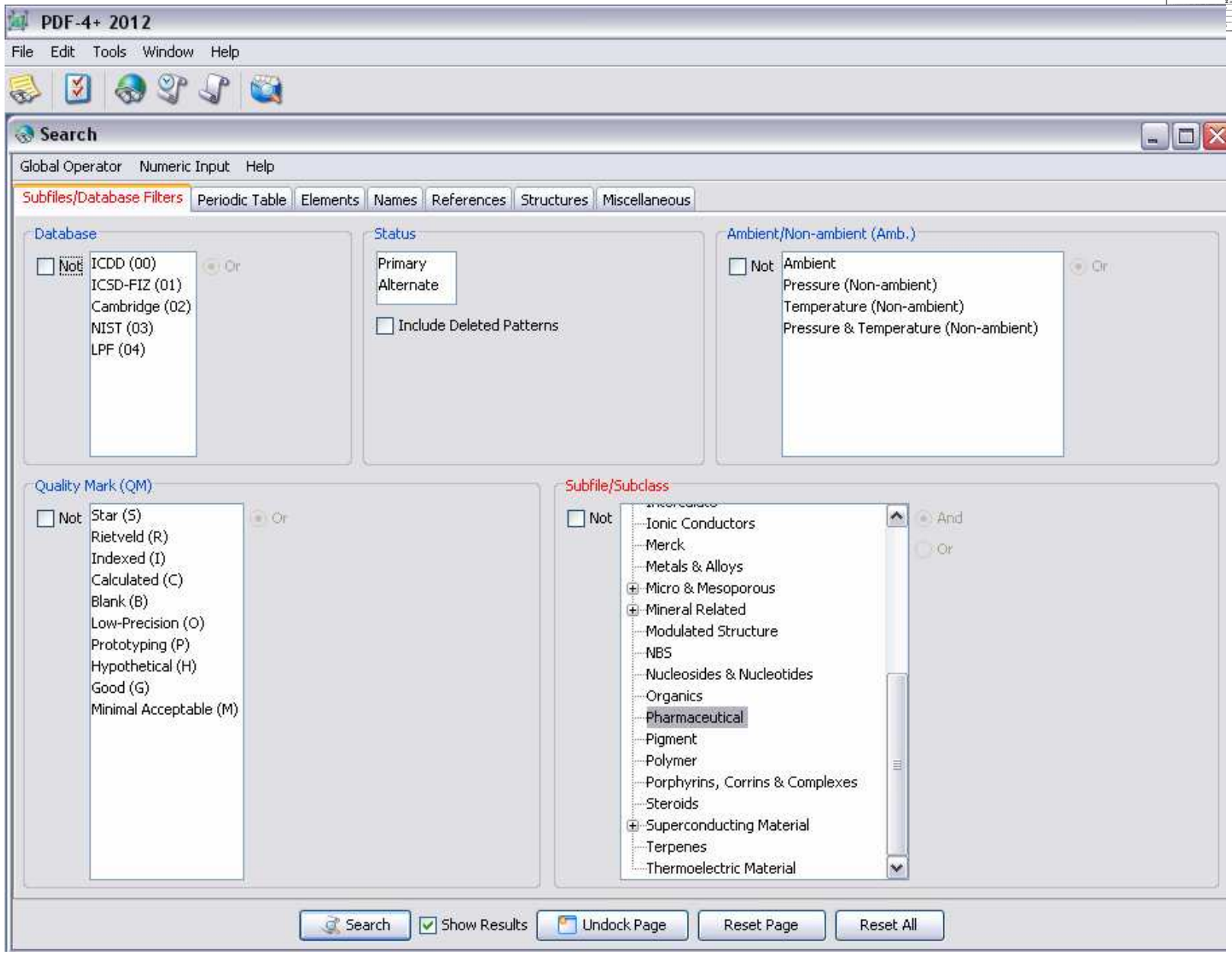


Example 1



- ✓Pharmaceutical phase
- ✓Ibuprofen




PDF-4+ 2012
File Edit Tools Window Help
Search
Global Operator Numeric Input Help
Subfiles/Database Filters Periodic Table Elements Names References Structures Miscellaneous
Database
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ICSD-FIZ (01)
Cambridge (02)
NIST (03)
LPF (04)
Or
Status
Primary
Alternate
Include Deleted Patterns
Ambient/Non-ambient (Amb.)
Not
Ambient
Pressure (Non-ambient)
Temperature (Non-ambient)
Pressure & Temperature (Non-ambient)
Or
Quality Mark (QM)
Not
Star (S)
Rietveld (R)
Indexed (I)
Calculated (C)
Blank (B)
Low-Precision (O)
Prototyping (P)
Hypothetical (H)
Good (G)
Minimal Acceptable (M)
Or
Subfile/Subclass
Not
Ionic Conductors
Merck
Metals & Alloys
Micro & Mesoporous
Mineral Related
Modulated Structure
NBS
Nucleosides & Nucleotides
Organics
Pharmaceutical
Pigment
Polymer
Porphyrins, Corrins & Complexes
Steroids
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Or
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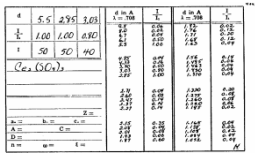
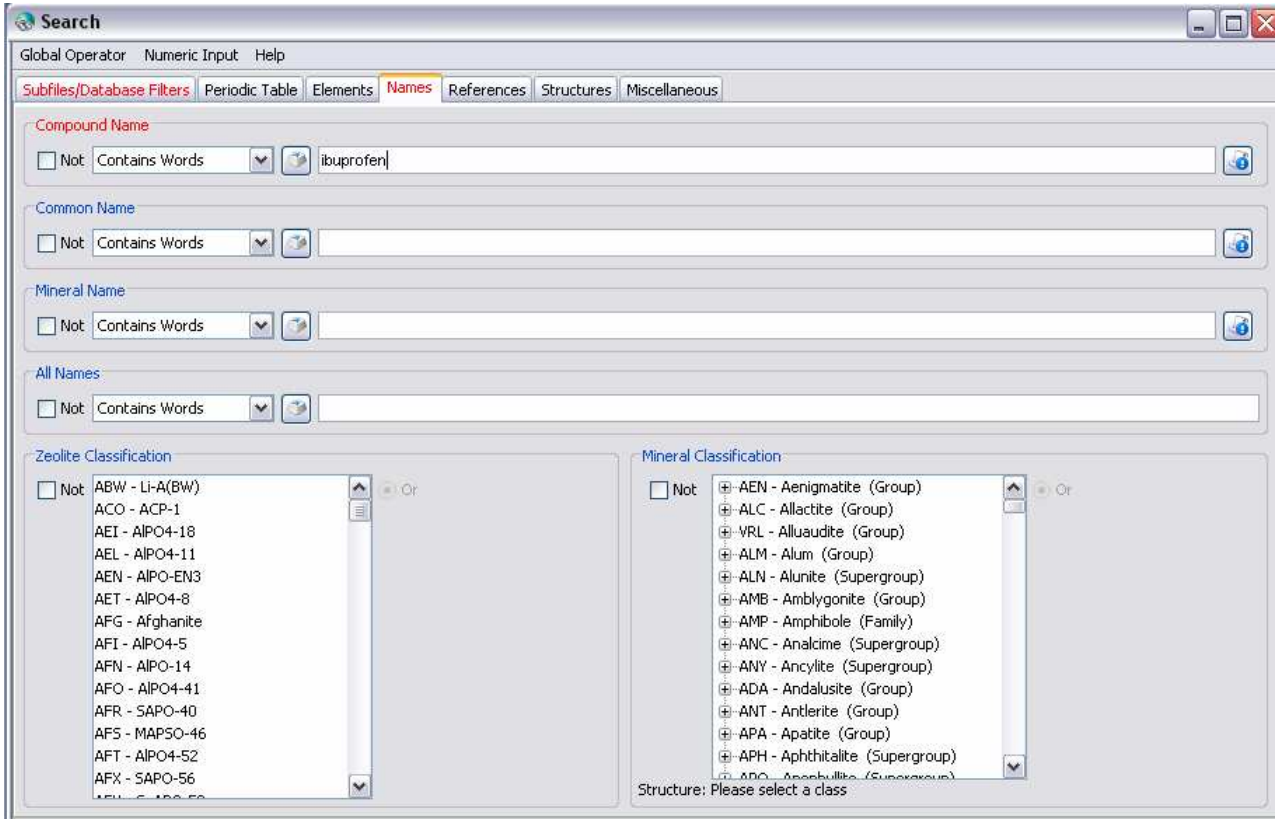
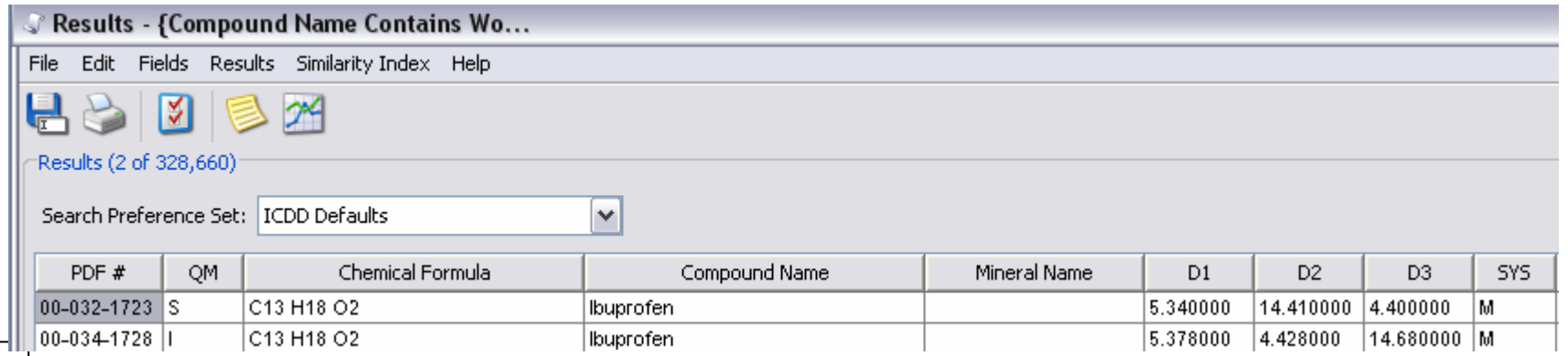
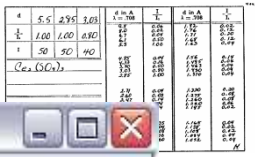






PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1	D2	D3	SYS
00-032-1723	S	C13 H18 O2	Ibuprofen		5.340000	14.410000	4.400000	M
00-034-1728	I	C13 H18 O2	Ibuprofen		5.378000	4.428000	14.680000	M



C13 H18 O2 - 00-032-1723

File Edit d-Spacings Tools Window Help

2D

d-Spacings

Wavelength

Cu Ka1 1.54056Å

Å

Stick Patterns

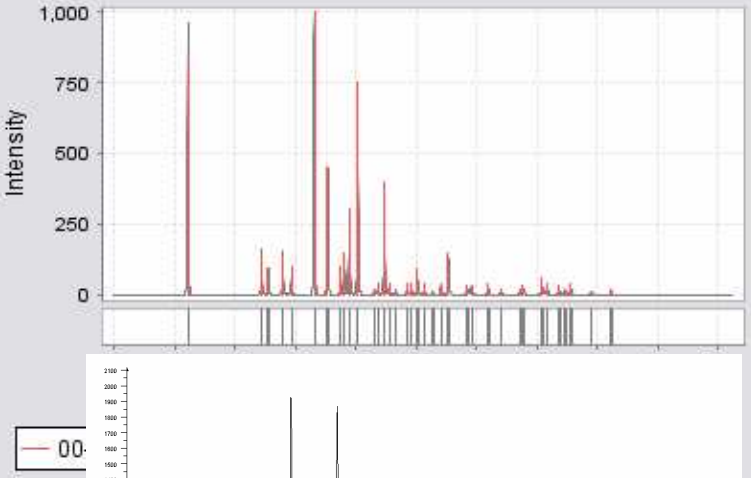
- [x] Fixed Slit Intensity
- [ ] Variable Slit Intensity
- [ ] Integrated Intensity

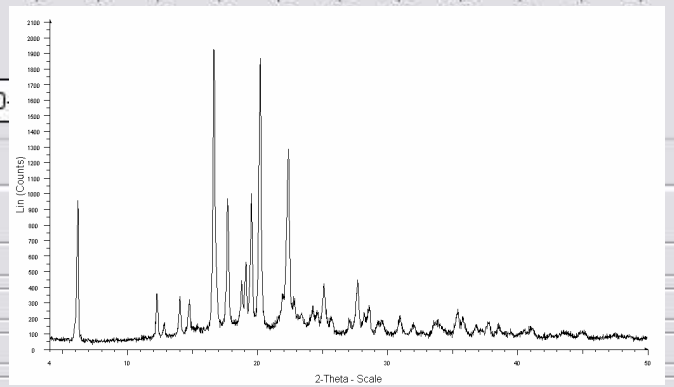
Diffraction Patterns

- [x] Simulated Profile
- [ ] Raw Diffraction Data (PD3)

Fixed Slit Intensity

2θ	d(Å)	I	h	k	l	*
6.1284	**14.410000**	85	1	0	0	
12.2148	7.240000	15	2	0	0	
12.7634	6.930000	9	1	1	0	
13.9790	6.330000	15	0	1	1	
14.7027	6.020000	10	-1	1	1	
16.5874	**5.340000**	100	2	1	0	
17.6884	5.010000	45	-2	1	1	
18.7447	4.730000	10	1	0	2	
19.0702	4.650000	15	-2	0	2	
19.4933	4.550000	30	2	1	1	
20.1647	**4.400000**	75	0	1	2	





PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

PDF #: 00-032-1723 Status: Primary

Pressure/Temperature: Ambient

Chemical Formula: C13 H18 O2

Structural Formula:

Empirical Formula: C13 H18 O2

Weight %: C75.69 H8.80 O15.51

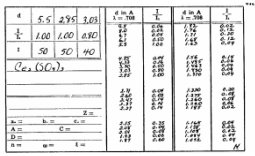
Atomic %: C39.39 H54.55 O6.06

ANX:

Compound Name: Ibuprofen

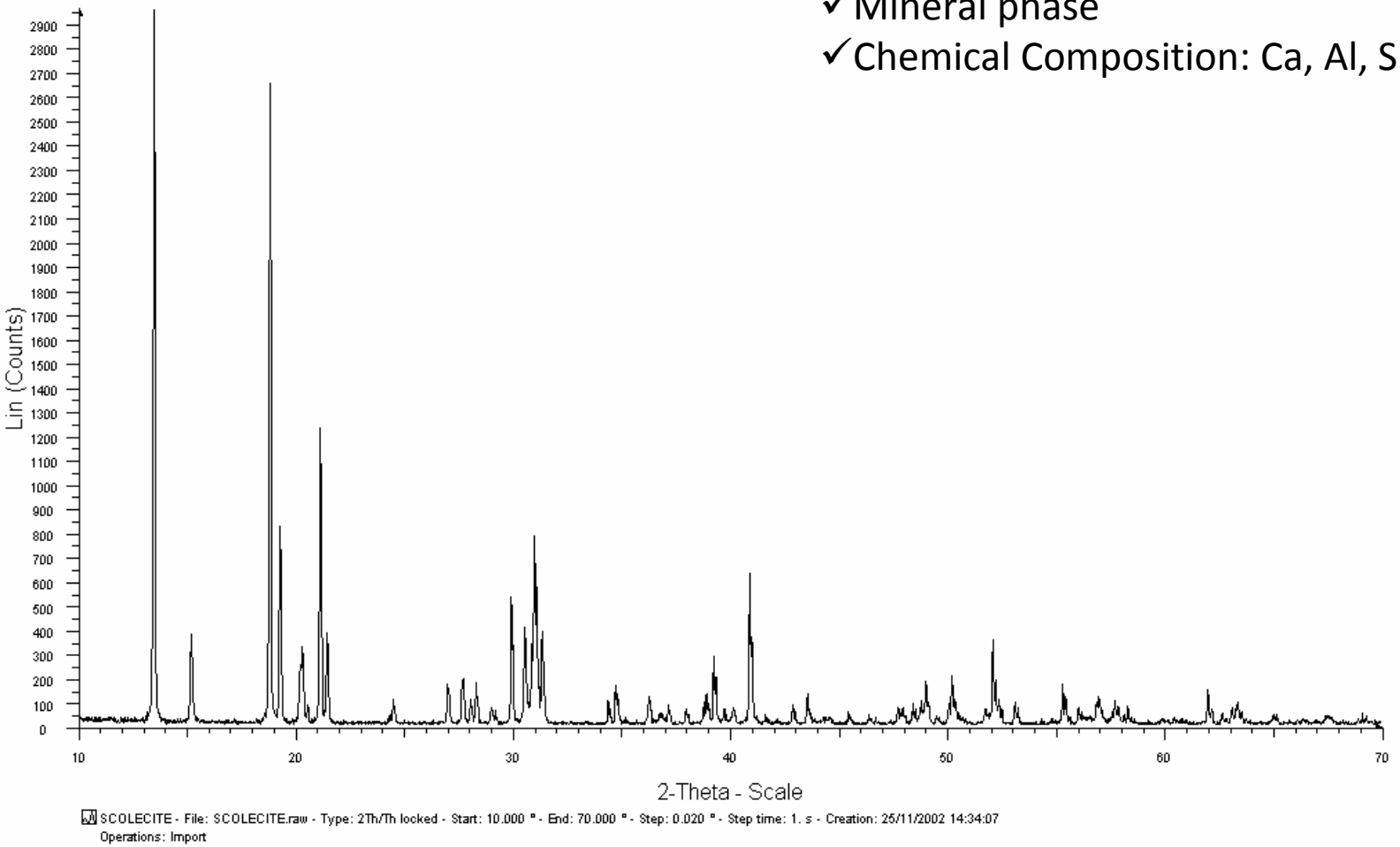
Mineral Name:

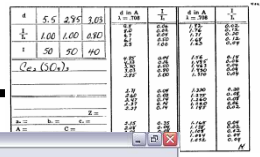
Common Name: 2-(4-(2-methylpropyl)phenyl)propanoic acid

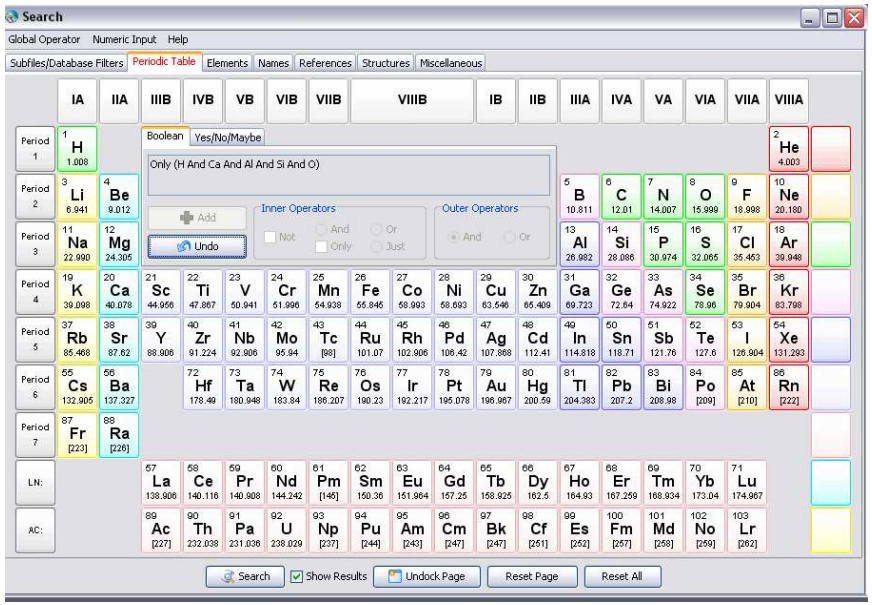


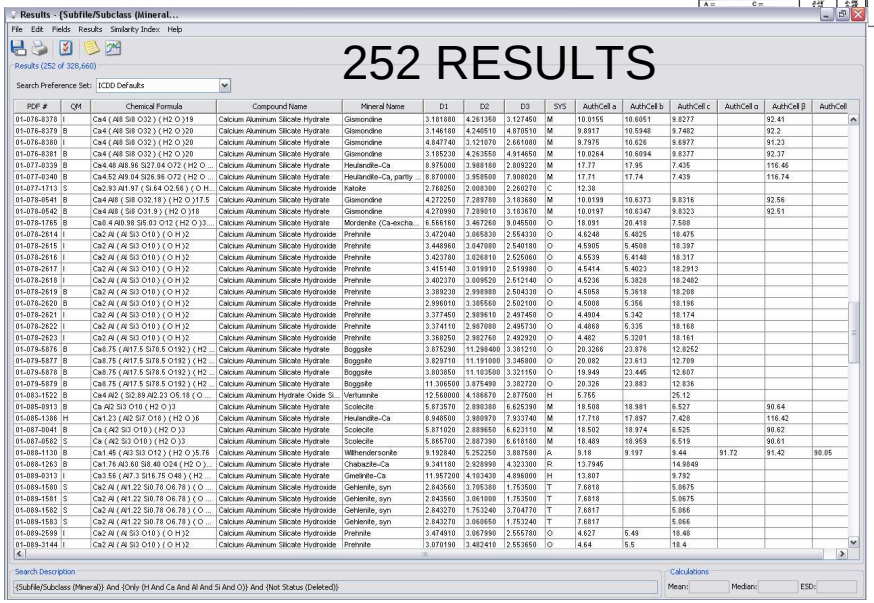
Example 2

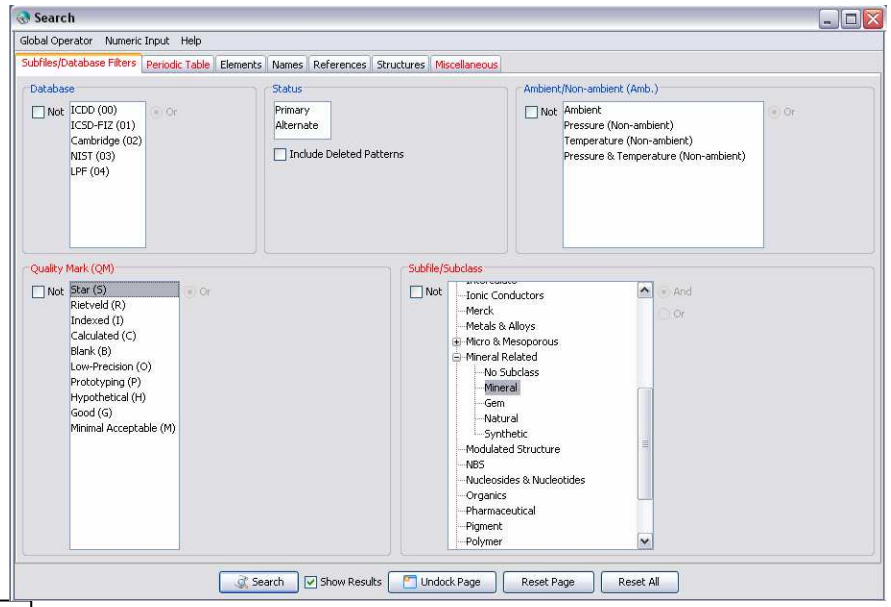
- ✓Mineral phase
- ✓Chemical Composition: Ca, Al, Si, O, H

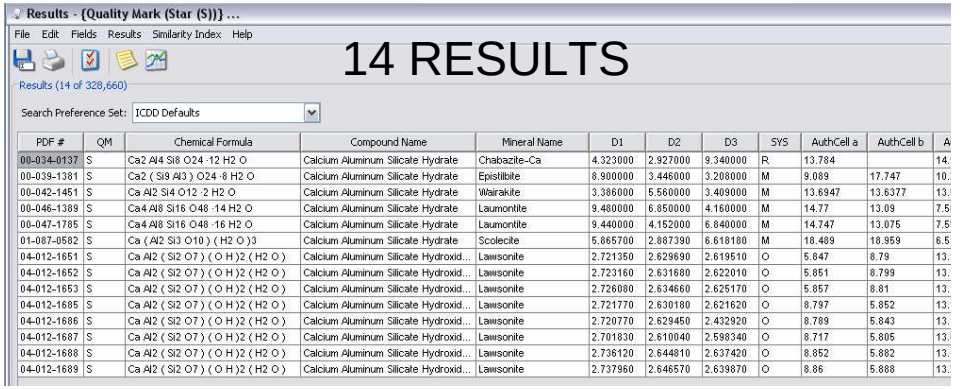




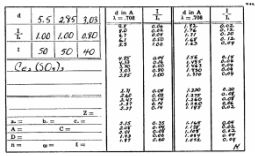


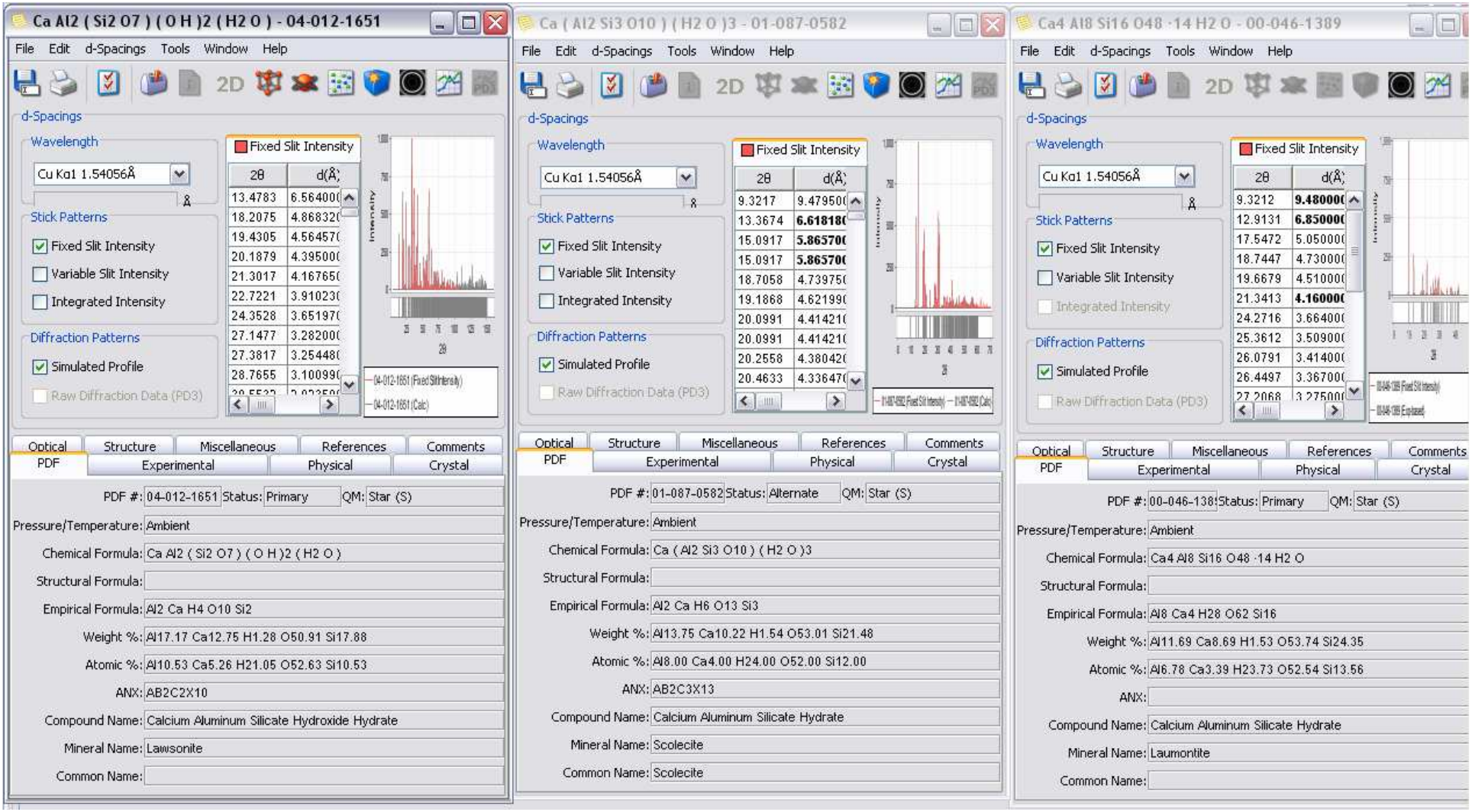






PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1	D2	D3	SYS	AuthCell a	AuthCell b	A
00-034-0137	S	Ca2 Al4 Si8 O24 ·12 H2 O	Calcium Aluminum Silicate Hydrate	Chabazite-Ca	4.323000	2.927000	9.340000	R	13.784		14.
00-039-1381	S	Ca2 (Si9 Al3) O24 ·8 H2 O	Calcium Aluminum Silicate Hydrate	Epistilbite	8.900000	3.446000	3.208000	M	9.089	17.747	10.
00-042-1451	S	Ca Al2 Si4 O12 ·2 H2 O	Calcium Aluminum Silicate Hydrate	Wairakite	3.386000	5.560000	3.409000	M	13.6947	13.6377	13.
00-046-1389	S	Ca4 Al8 Si16 O48 ·14 H2 O	Calcium Aluminum Silicate Hydrate	Laumontite	9.480000	6.850000	4.160000	M	14.77	13.09	7.5
00-047-1785	S	Ca4 Al8 Si16 O48 ·16 H2 O	Calcium Aluminum Silicate Hydrate	Laumontite	9.440000	4.152000	6.840000	M	14.747	13.075	7.5
01-087-0562	S	Ca (Al2 Si3 O10) (H2 O)3	Calcium Aluminum Silicate Hydrate	Scolecite	5.865700	2.887390	6.618180	M	18.489	18.959	6.5
04-012-1651	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.721350	2.629690	2.619510	O	5.847	8.79	13.
04-012-1652	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.723160	2.631680	2.622010	O	5.851	8.799	13.
04-012-1653	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.726080	2.634660	2.625170	O	5.857	8.81	13.
04-012-1685	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.721770	2.630180	2.621620	O	8.797	5.852	13.
04-012-1686	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.720770	2.629450	2.432920	O	8.789	5.843	13.
04-012-1687	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.701830	2.610040	2.598340	O	8.717	5.805	13.
04-012-1688	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.736120	2.644810	2.637420	O	8.852	5.882	13.
04-012-1689	S	Ca Al2 (Si2 O7) (O H)2 (H2 O)	Calcium Aluminum Silicate Hydroxid...	Lawsonite	2.737960	2.646570	2.639870	O	8.86	5.888	13.




Ca Al2 (Si2 O7) (O H)2 (H2 O) - 04-012-1651
File Edit d-Spacings Tools Window Help
d-Spacings
Wavelength
Cu Kα1 1.54056Å
Stick Patterns
Fixed Slit Intensity
Variable Slit Intensity
Integrated Intensity
Diffraction Patterns
Simulated Profile
Raw Diffraction Data (PD3)
Fixed Slit Intensity
2θ d(Å)
13.4783 6.56400
18.2075 4.86832
19.4305 4.56457
20.1879 4.39500
21.3017 4.16765
22.7221 3.91023
24.3528 3.65197
27.1477 3.28200
27.3817 3.25448
28.7655 3.10099
Optical Structure Miscellaneous References Comments
PDF Experimental Physical Crystal
PDF #: 04-012-1651 Status: Primary QM: Star (S)
Pressure/Temperature: Ambient
Chemical Formula: Ca Al2 (Si2 O7) (O H)2 (H2 O)
Structural Formula:
Empirical Formula: Al2 Ca H4 O10 Si2
Weight %: Al17.17 Ca12.75 H1.28 O50.91 Si17.88
Atomic %: Al10.53 Ca5.26 H21.05 O52.63 Si10.53
ANX: AB2C2X10
Compound Name: Calcium Aluminum Silicate Hydroxide Hydrate
Mineral Name: Lawsonite
Common Name:
Ca (Al2 Si3 O10) (H2 O)3 - 01-087-0582
File Edit d-Spacings Tools Window Help
d-Spacings
Wavelength
Cu Kα1 1.54056Å
Stick Patterns
Fixed Slit Intensity
Variable Slit Intensity
Integrated Intensity
Diffraction Patterns
Simulated Profile
Raw Diffraction Data (PD3)
Fixed Slit Intensity
2θ d(Å)
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13.3674 6.61818
15.0917 5.86570
15.0917 5.86570
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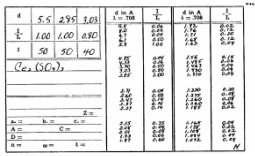
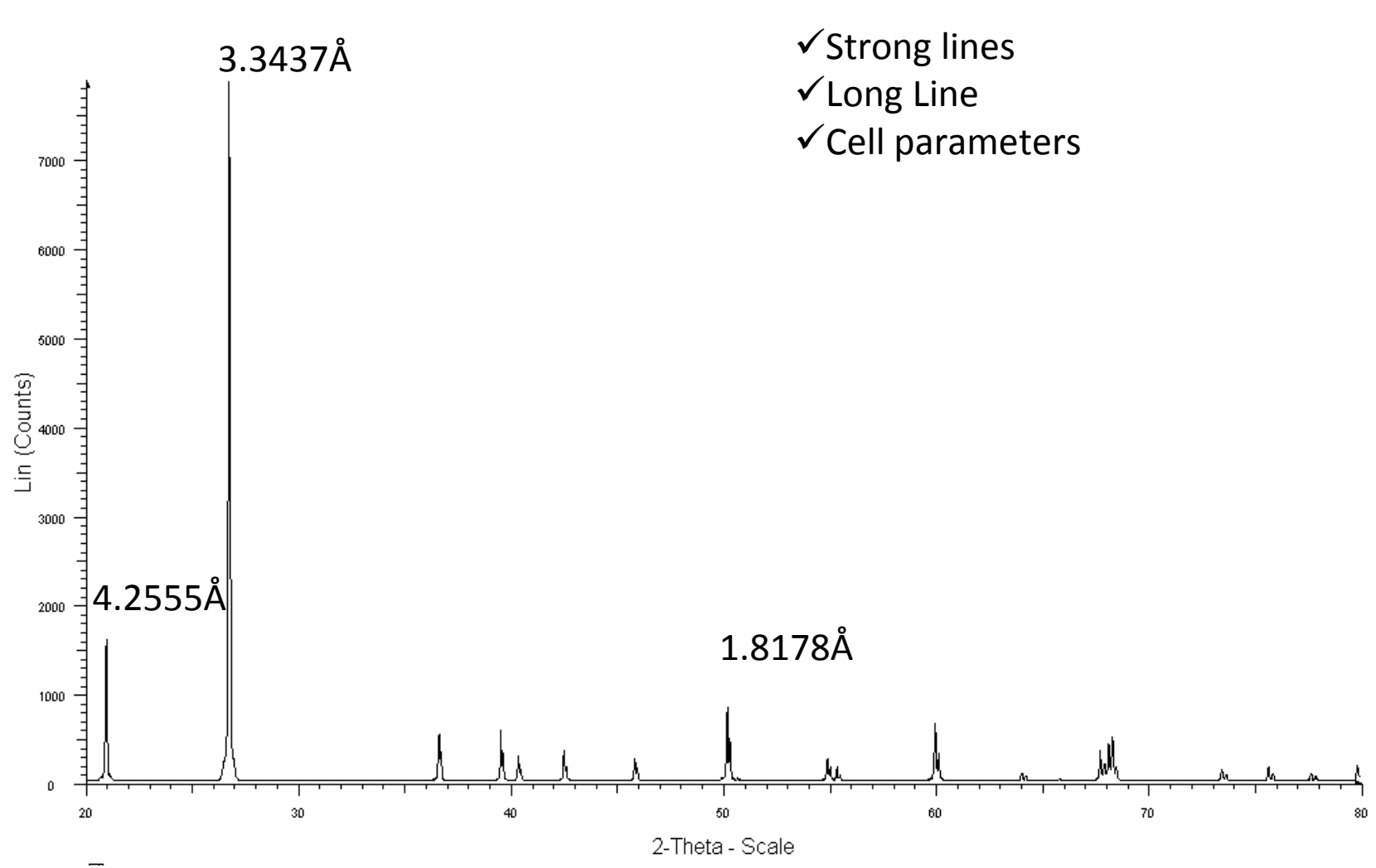
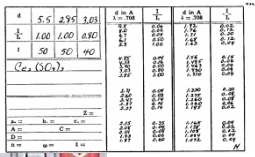
19.1868 4.62199
20.0991 4.41421
20.0991 4.41421
20.2558 4.38042
20.4633 4.33647
Optical Structure Miscellaneous References Comments
PDF Experimental Physical Crystal
PDF #: 01-087-0582 Status: Alternate QM: Star (S)
Pressure/Temperature: Ambient
Chemical Formula: Ca (Al2 Si3 O10) (H2 O)3
Structural Formula:
Empirical Formula: Al2 Ca H6 O13 Si3
Weight %: Al13.75 Ca10.22 H1.54 O53.01 Si21.48
Atomic %: Al8.00 Ca4.00 H24.00 O52.00 Si12.00
ANX: AB2C3X13
Compound Name: Calcium Aluminum Silicate Hydrate
Mineral Name: Scolecite
Common Name: Scolecite
Ca4 Al8 Si16 O48 ·14 H2 O - 00-046-1389
File Edit d-Spacings Tools Window Help
d-Spacings
Wavelength
Cu Kα1 1.54056Å
Stick Patterns
Fixed Slit Intensity
Variable Slit Intensity
Integrated Intensity
Diffraction Patterns
Simulated Profile
Raw Diffraction Data (PD3)
Fixed Slit Intensity
2θ d(Å)
9.3212 9.48000
12.9131 6.85000
17.5472 5.05000
18.7447 4.73000
19.6679 4.51000
21.3413 4.16000
24.2716 3.66400
25.3612 3.50900
26.0791 3.41400
26.4497 3.36700
Optical Structure Miscellaneous References Comments
PDF Experimental Physical Crystal
PDF #: 00-046-138 Status: Primary QM: Star (S)
Pressure/Temperature: Ambient
Chemical Formula: Ca4 Al8 Si16 O48 ·14 H2 O
Structural Formula:
Empirical Formula: Al8 Ca4 H28 O62 Si16
Weight %: Al11.69 Ca8.69 H1.53 O53.74 Si24.35
Atomic %: Al6.78 Ca3.39 H23.73 O52.54 Si13.56
ANX:
Compound Name: Calcium Aluminum Silicate Hydrate
Mineral Name: Laumontite
Common Name:



Example 3



- ✓Strong lines
- ✓Long Line
- ✓Cell parameters



Search

Global Operator | Numeric Input | Help

Subfiles/Database Filters | Periodic Table | Elements | Names | References | Structures | Miscellaneous

Long Line

Not 4.2555 Å ESD: 0.3 Å L1 L2 L3

Not g/cm³ ESD: g/cm³ Dcalc Dstruc

Melting Point

Not ESD: °C °K °F

Color

Not Black, Blue, Brown, Color Missing, Colorless, Gray, Green — And / Or

Strong Line

Not 3.3437 Å ESD: 0.3 Å D1 D2 D3

Strong Line

Not 4.2555 Å ESD: 0.3 Å D1 D2 D3

Strong Line

Not 1.8178 Å ESD: 0.3 Å D1 D2 D3

Organic F

Not >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) — And / Or

Smith-Snyder Figure Of Merit (SS/FOM)

Not ESD:

Has PD3 Pattern

Yes No

Has Property Sheet

Yes No

Database Comments

Not Contains Words

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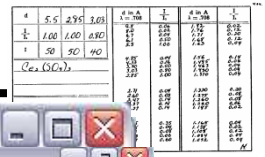

Search

Results - {Crystal Data a = 4.914(0....

File Edit Fields Results Similarity Index Help

Results (82 of 328,660)

Search Preference Set: ICDD Defaults

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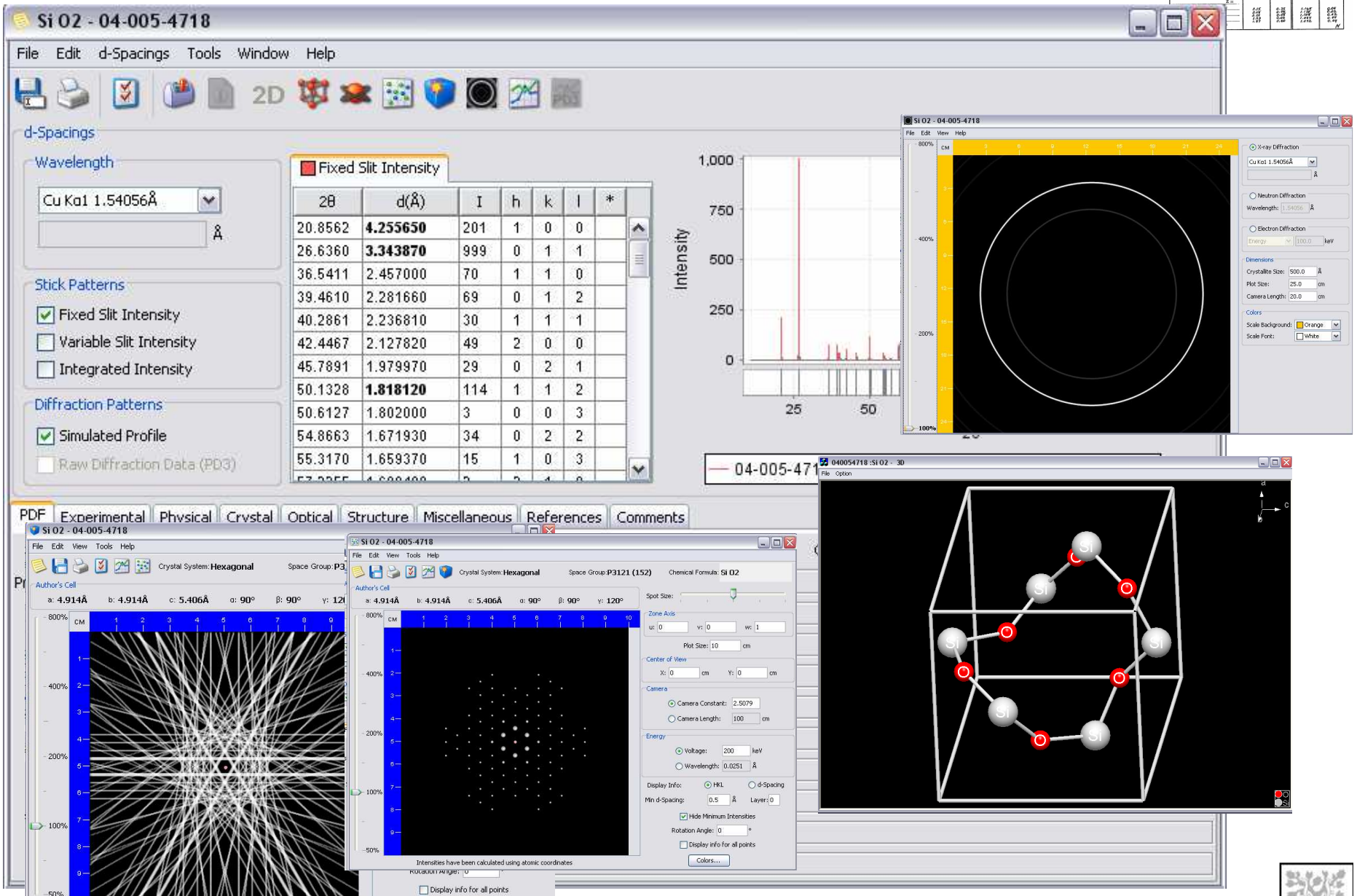
01-085-0865	I	Si O2	Silicon Oxide	Quartz, syn	3.336560	4.243520	1.814370	H	4.9		5.4			
01-085-0930	S	Si O2	Silicon Oxide	Quartz, syn	3.342840	4.253050	1.817670	H	4.911		5.407			
01-085-1053	I	Si O2	Silicon Oxide	Quartz, syn	3.342940	4.254610	1.817610	H	4.9128		5.4042			
01-085-1054	S	Si O2	Silicon Oxide	Quartz	3.343530	4.255390	1.817930	H	4.9137		5.4051			
01-086-1560	S	Si O2	Silicon Oxide	Quartz	3.344560	4.257380	1.818440	H	4.916		5.4054			
01-086-1628	S	Si O2	Silicon Oxide	Quartz, syn	3.337370	4.245340	1.814750	H	4.9021		5.3997			
01-086-1629	S	Si O2	Silicon Oxide	Quartz, syn	3.337800	4.246120	1.814970	H	4.903		5.3999			
01-086-1630	S	Si O2	Silicon Oxide	Quartz, syn	3.343910	4.255740	1.818140	H	4.9141		5.406			
01-086-2237	I	Si O2	Silicon Oxide	Quartz	3.342970	4.254780	1.817620	H	4.913		5.404			
01-087-2096	S	Si O2	Silicon Oxide	Quartz low, syn	3.342960	4.254520	1.817630	H	4.9127		5.4045			
01-088-2487	H	Si O2	Silicon Oxide	Quartz, syn	3.345560	4.269510	1.818140	H	4.93		5.385			
01-089-1961	I	Si O2	Silicon Oxide	Quartz low, syn	3.349170	4.261710	1.821060	H	4.921		5.416			
01-089-8934	S	Si O2	Silicon Oxide	Quartz	3.343430	4.255390	1.817870	H	4.9137		5.4047			
01-089-8935	S	Si O2	Silicon Oxide		3.347500	4.261620	1.819990	H	4.9209		5.4091			
01-089-8936	S	Si O2	Silicon Oxide		3.352610	4.269250	1.822690	H	4.9297		5.4151			
01-089-8937	S	Si O2	Silicon Oxide		3.357730	4.276780	1.825390	H	4.9384		5.4213			
01-089-8938	S	Si O2	Silicon Oxide		3.364680	4.287610	1.829020	H	4.9509		5.4285			
01-089-8939	S	Si O2	Silicon Oxide		3.371450	4.297910	1.832560	H	4.9628		5.436			
03-065-0466	I	O2 Si	Silicon Oxide	Quartz low, syn	3.343910	4.255740	1.818140	H	4.9141		5.406			
04-001-9367	P	Si O2	Silicon Oxide		3.340770	4.252180	1.816400	H	4.91		5.4			
04-002-3600	P	Si O2	Silicon Oxide	Quartz	3.343280	4.255130	1.817790	H	4.9134		5.4046			
04-003-6495	P	Si O2	Silicon Oxide	Quartz	3.343450	4.254780	1.817920	H	4.913		5.406			
04-005-4494	B	Si O2	Silicon Oxide	Quartz, syn	3.342680	4.254250	1.817470	H	4.9124		5.4039			
04-005-4718	S	Si O2	Silicon Oxide	Quartz, syn	3.343870	4.255650	1.818120	H	4.914		5.406			
04-006-1757	P	Si O2	Silicon Oxide	Quartz	3.337820	4.246120	1.814980	H	4.903		5.4			
04-006-5050	P	Si O2	Silicon Oxide		3.343000	4.254700	1.817640	H	4.9129		5.4043			
04-007-5142	P	Si O2	Silicon Oxide	quartz	3.343270	4.254960	1.817790	H	4.9132		5.4049			
04-007-9911	P	Si O2	Silicon Oxide	quartz low	3.342470	4.254180	1.817340	H	4.9123		5.4031			
04-008-2359	P	Si O2	Silicon Oxide	quartz low	3.342940	4.254520	1.817620	H	4.9127		5.4044			
04-008-4810	I	Ge0.14 Si0.86 O2	Germanium Silicon Oxide	Quartz, germanian, syn	3.372230	4.294620	1.833330	H	4.959		5.446			
04-008-7651	I	Si O2	Silicon Oxide	Quartz	3.344250	4.256340	1.818320	H	4.9148		5.4062			
04-008-7652	I	Si O2	Silicon Oxide	quartz low	3.344280	4.256260	1.818340	H	4.9147		5.4065			
04-008-7653	I	Si O2	Silicon Oxide	quartz low	3.330030	4.235900	1.810760	H	4.8912		5.388			
04-008-7654	I	Si O2	Silicon Oxide	quartz low	3.316550	4.216760	1.803590	H	4.8691		5.3703			
04-008-7655	I	Si O2	Silicon Oxide	quartz low	3.314940	4.215640	1.802640	H	4.8678		5.3658			
04-008-8228	P	Si O2	Silicon Oxide	quartz low	3.342810	4.254350	1.817550	H	4.9125		5.4042			
04-012-0490	I	Si O2	Silicon Oxide	Quartz	3.343930	4.255880	1.818150	H	4.9143		5.4058			
04-014-3910	I	Be0.94 F1.88	Beryllium Fluoride		3.331830	2.229690	1.811330	H	4.9		5.38			

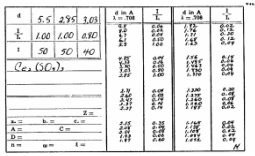
Search Description

{Crystal Data a = 4.914(0.05)Å And Crystal Data b = 4.914(0.05)Å And Crystal Data c = 5.406(0.05)Å} And {Long Line = 4.2555(0.3)Å} And {Not Status (Deleted)}

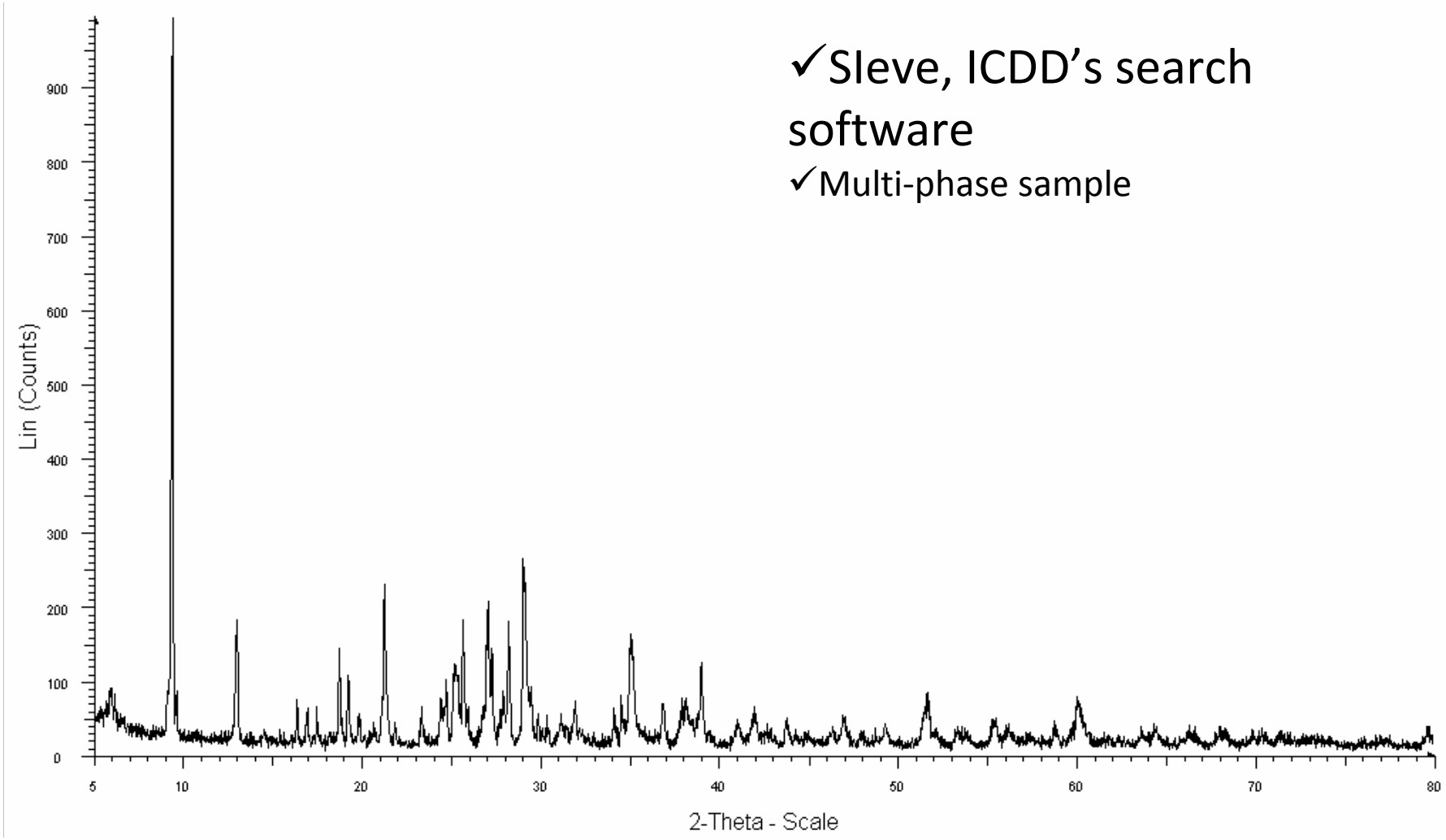
Calculations

Mean: Median: ESD:


Si O2 - 04-005-4718
File Edit d-Spacings Tools Window Help
d-Spacings
Wavelength
Cu Ka1 1.54056Å
Å
Stick Patterns
Fixed Slit Intensity
Variable Slit Intensity
Integrated Intensity
Diffraction Patterns
Simulated Profile
Raw Diffraction Data (PD3)
Fixed Slit Intensity
2θ d(Å) I h k l *
20.8562 4.255650 201 1 0 0
26.6360 3.343870 999 0 1 1
36.5411 2.457000 70 1 1 0
39.4610 2.281660 69 0 1 2
40.2861 2.236810 30 1 1 1
42.4467 2.127820 49 2 0 0
45.7891 1.979970 29 0 2 1
50.1328 1.818120 114 1 1 2
50.6127 1.802000 3 0 0 3
54.8663 1.671930 34 0 2 2
55.3170 1.659370 15 1 0 3
Intensity
1,000
750
500
250
0
25
50
PDF Experimental Physical Crystal Optical Structure Miscellaneous References Comments
Crystal System: Hexagonal
Space Group: P3121 (152)
Chemical Formula: Si O2
Author's Cell
a: 4.914Å b: 4.914Å c: 5.406Å α: 90° β: 90° γ: 120°
Intensities have been calculated using atomic coordinates
Display info for all points
Colors...

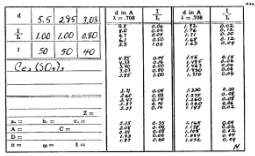


Example 4

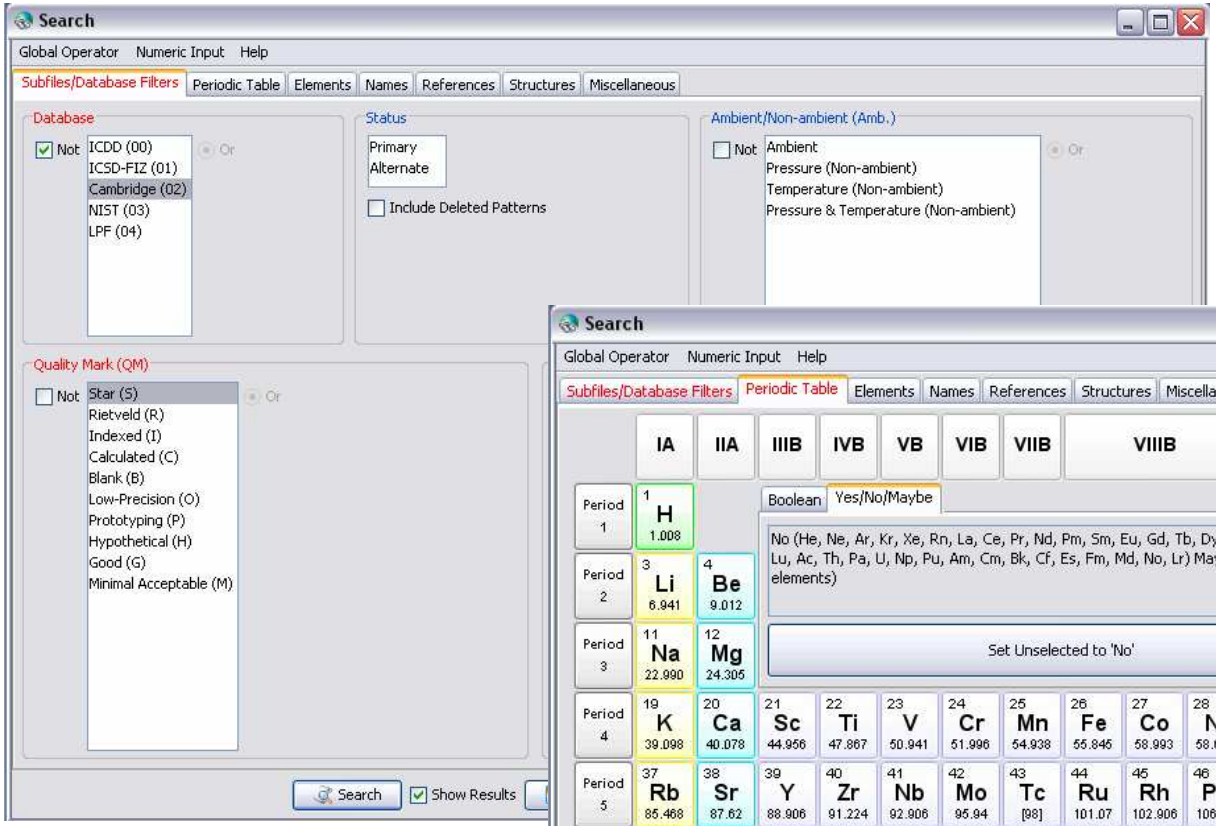


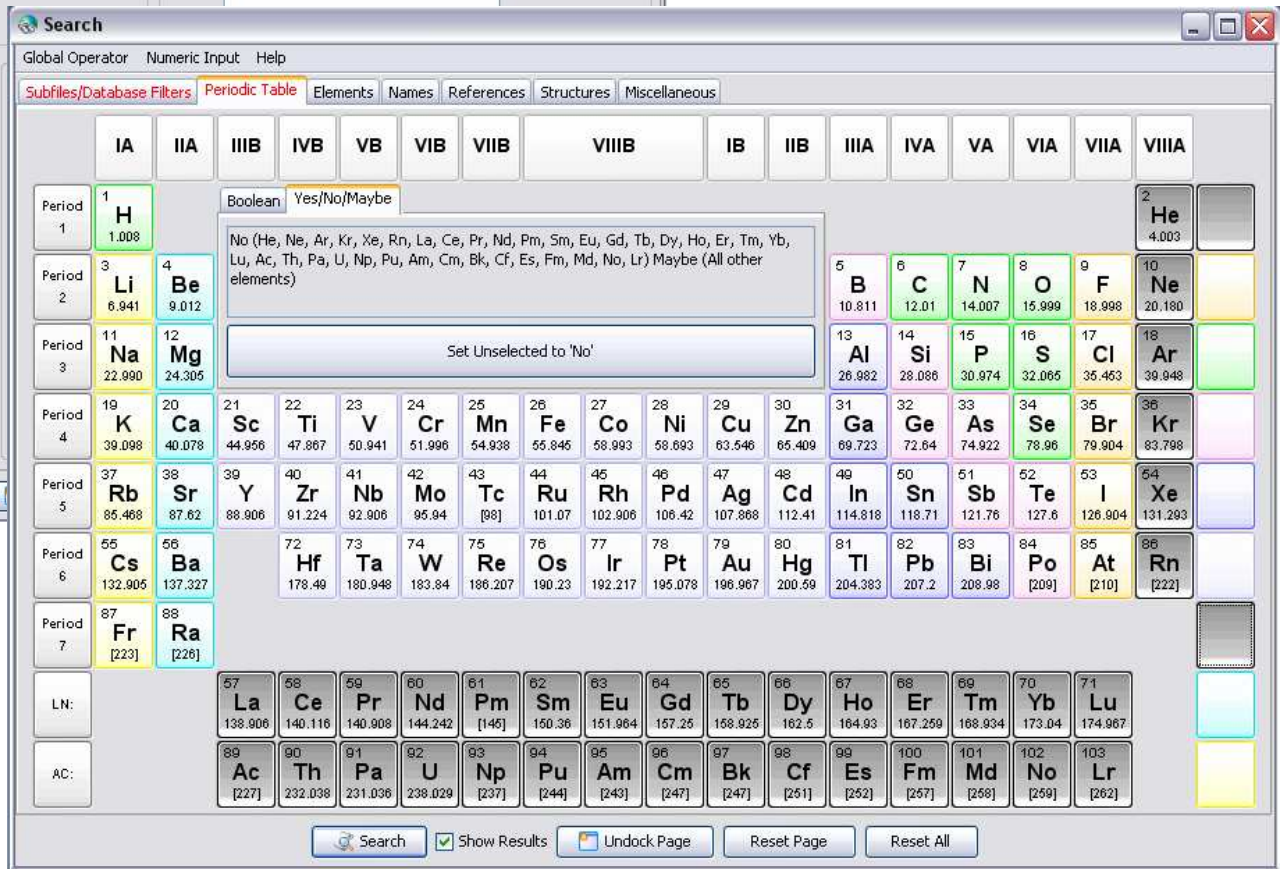
✓SIeve, ICDD's search software

✓Multi-phase sample

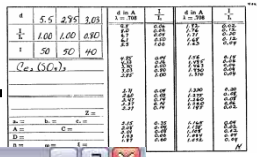


Step 1


Search
Global Operator
Numeric Input
Help
Subfiles/Database Filters
Periodic Table
Elements
Names
References
Structures
Miscellaneous
Database
Not
ICDD (00)
ICSD-FIZ (01)
Cambridge (02)
NIST (03)
LPF (04)
Or
Status
Primary
Alternate
Include Deleted Patterns
Ambient/Non-ambient (Amb.)
Not
Ambient
Pressure (Non-ambient)
Temperature (Non-ambient)
Pressure & Temperature (Non-ambient)
Quality Mark (QM)
Not
Star (S)
Rietveld (R)
Indexed (I)
Calculated (C)
Blank (B)
Low-Precision (O)
Prototyping (P)
Hypothetical (H)
Good (G)
Minimal Acceptable (M)
Search
Show Results


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
Boolean
Yes/No/Maybe
No (He, Ne, Ar, Kr, Xe, Rn, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) Maybe (All other elements)
Set Unselected to 'No'
Search
Show Results
Undock Page
Reset Page
Reset All


Sleve+ - (Untitled)
Matches Filter
Past Search Filters
Name
Description
Hits
Search #1
{Not Database (Cambridge (02))} And {Quality Mark (Star (S))} And {Subfile/Subclass (Mineral)} And {No (He, Ne, Ar, Kr, Xe, Rn, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) Maybe (All other
5,809
Step 2
Or
Common Filters
Primary Patterns
Mineral Related
Pharmaceuticals and Excipients
Common Phases
Apply Filter
No Filter
No Filter But Exclude Deleted
Cancel
Intensity
2θ
Manual Peak Selection
Add
Remove
Off
Process Data
Import
Advanced Mode
Cancel



Sleve+ - Sara000.xml

File Edit Matches Phases Lines Help

Phase 1 Phase 2 Phase 3

Matches (83 of 5,809)

GOM	PDF #	QM	Status	Coords	Compound Name	Chemical Formula	LS1	LS2	LS3	LS4	LS5	LS6	LS7	LS8	I/Ic	Rot. #
2103	04-014-9934	I	P	✓	Calcium Aluminum Silicon Oxide Chlo...	Ca Al1.8 Si3.2 Cl0.2 O8 (O H)4 (H...	9.776120	5.434760	4.888060	4.716310	4.070480	3.816690	3.605090	3.175880	0.76	
3067	00-007-0017	S	P	✓	Potassium Aluminum Sulfate Hydrate	K Al (S O4)2 ·12 H2 O	5.440000	4.960000	4.298000	4.053000	3.250000	3.039000	2.950000	2.866000		2
2537	00-011-0699	S	P	✓	Iron Arsenide	Fe As2	2.605000	2.599000	2.532000	2.421000	2.331000	1.867000	1.854300	1.694500		8
2310	00-022-0153	S	P	✓	Calcium Titanium Oxide	Ca Ti O3	3.824000	2.719000	2.701000	2.303000	1.911000	1.567000	1.563000	1.557000	2.6	6
4168	00-024-0719	S	P	✓	Magnesium Sulfate Hydrate	Mg S O4 ·6 H2 O	5.450000	5.100000	4.880000	4.390000	4.160000	4.040000	3.610000	3.197000		2
3912	00-031-0297	S	A	✓	Calcium Silicate	Ca2 Si O4	4.317000	3.818000	3.379000	3.012000	2.895000	2.750000	2.729000	1.908500		4
2028	00-034-0415	S	P	✓	Zirconium Titanium Oxide	Zr Ti O4	3.613890	2.933900	2.743550	2.516950	2.153820	1.854250	1.806740	1.737560		7
3137	00-035-0424	S	P	✓	Sodium Aluminum Silicate	Na Al Si O4	4.321000	4.165000	3.834000	3.266000	3.040000	3.000000	2.881000	2.570000		4
2667	00-041-1472	S	P	✓	Nickel Antimony Sulfide	Ni Sb S	4.193000	3.424000	2.965000	2.653000	2.421000	1.788700	1.645100	1.585400		5
2553	00-047-1738	S	P	✓	Cobalt Sulfide	Co3 S4	5.444000	3.331000	2.841000	2.356000	1.923600	1.813500	1.665600	1.436900		2

Change Filter...

Filter Description

{Not Database (Cambridge (02))} And {Quality Mark (Star (S))} And {Subfile/Subclass (Mineral)} And {No (He, Ne, Ar, Kr, Xe, Rn, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) Maybe (All other elements)} And {Not Status (Deleted)}

Experiment

Search Line(s): 15.06930 Å D1 Range: 14.684 - 15.455 Å Rotation: All

Preferences

Search Method: Long8 Wavelength: Cu Ka1 1.54056Å

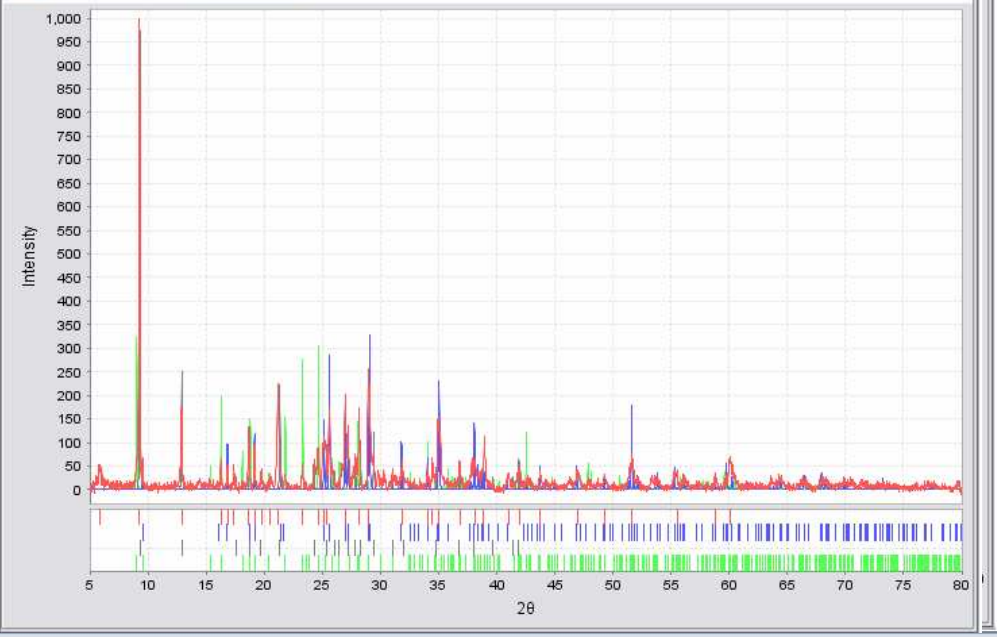
Search Window: 0.15 ° Match Window: 0.15 °

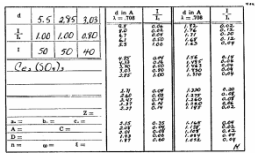
Lowest Allowable GOM: 2000 ☑ Weight d-Spacings

Phases (3)

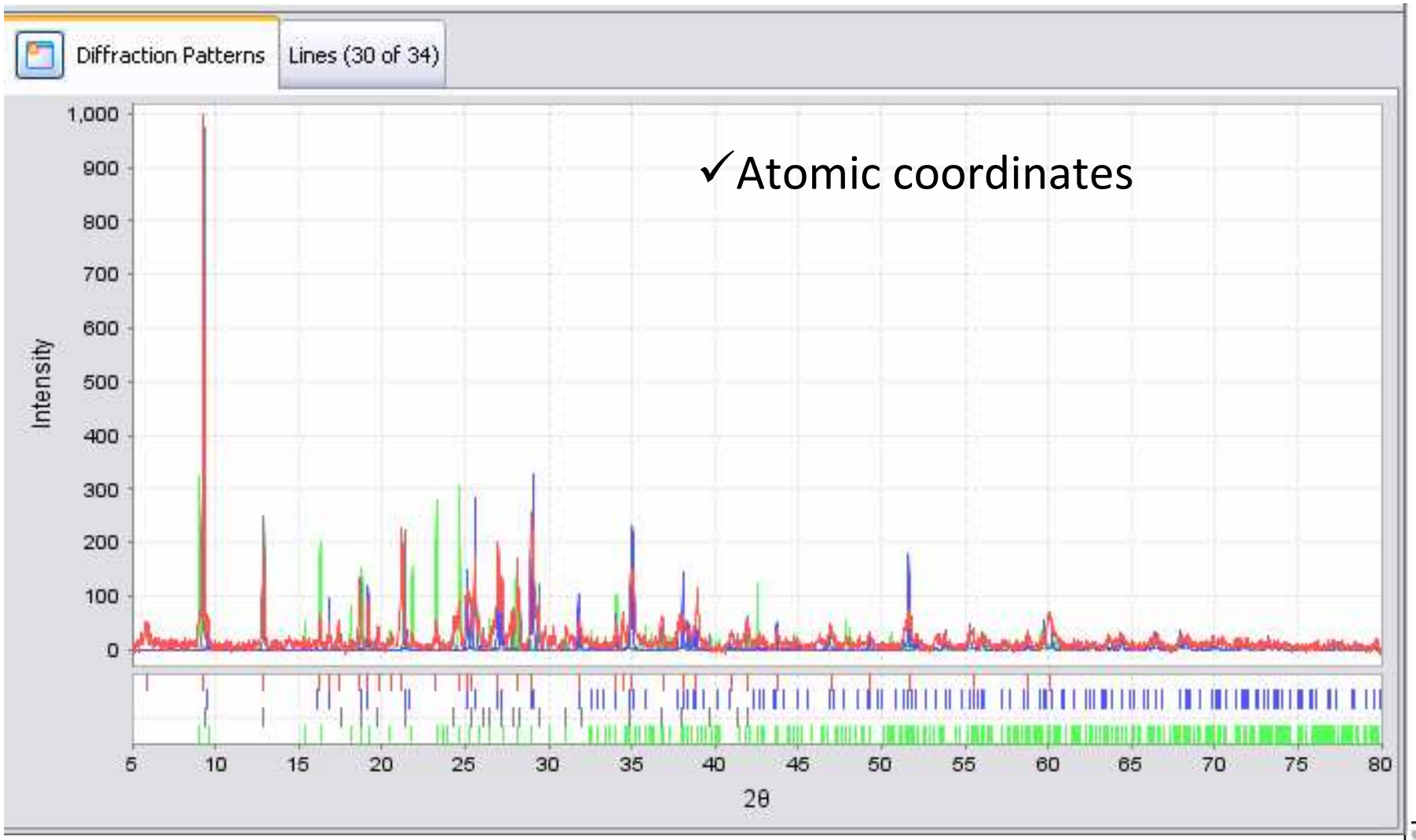
#		PDF #	Compound Name	I Ratio	I %	I/Ic	Est Wt %
1	✓	04-015-8389	Calcium Aluminum Iron Silicate Hydr...	0.329	20	0.68*	
2	✓	00-046-1389	Calcium Aluminum Silicate Hydrate	0.973	60		
3		04-014-9934	Calcium Aluminum Silicon Oxide Chlo...	0.323	20	0.76	

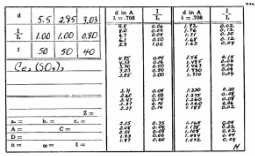
Diffraction Patterns Lines (30 of 34)





Example 5


Diffraction Patterns
Lines (30 of 34)
✓Atomic coordinates
Intensity
1,000
900
800
700
600
500
400
300
200
100
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
2θ



Ca2 Fe0.26 Al1.74 Si3 O10 (O H

04-015-8389 Mar 28, 2013 10:17 AM (jgil)

Status Alternate QM: Star (S) Pressure/Temperature: Ambient
Chemical Formula: Ca2 Fe0.26 Al1.74 Si3 O10 (O H)2 Empirical Formula: Al1.74 Ca2 Fe0.26 H2 O12 Si3
Weight %: Al11.18 Ca19.09 Fe3.46 H0.48 O45.72 Si20.07 Atomic %: Al8.29 Ca9.52 Fe1.24 H9.52 O57.14 Si14.29

File Edit d-Spacings Tools Window

Save

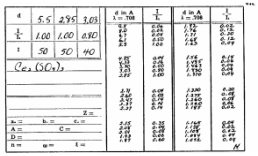
Structure

Atomic Coordinates

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	IDP	AET
Ca	1	4d	1	0.0051	1.23913	0.84931	1.0	0.00933	
Al	2	2c	..m	0.0026	0.73772	0.75	0.72	0.00633	
Fe	3	2c	..m	0.0026	0.73772	0.75	0.28	0.00633	
Si	4	4d	1	0.4964	0.74899	0.86953	1.0	0.0060	
Al	5	2b	2..	0.1888	1.0	1.0	1.0	0.00633	
Si	6	2a	2..	-0.194	1.5	1.5	1.0	0.00633	
O	7	4d	1	0.7544	0.8701	0.8234	1.0	0.0090	
O	8	4d	1	0.2538	1.6060000000000003	1.6767	1.0	0.0090	
O	9	4d	1	0.3573	0.97	0.91728	1.0	0.01067	
O	10	4d	1	0.6207	1.5392999999999997	1.57418	1.0	0.01067	
O	11	4d	1	-0.0096	0.7398	1.0197	1.0	0.01167	
O	12	2c	..m	0.2095	1.04	0.75	1.0	0.00833	
O	13	2c	..m	0.7973	1.4363	0.75	1.0	0.00833	
H	14	2c	..m	0.4	1.0039999999999998	0.75	1.0	0.035	
H	15	2c	..m	0.605	1.4610000000000003	0.75	1.0	0.035	

Atomic %: Al8.29 Ca
ANX:
Compound Name: Calcium A
Mineral Name: prehnite
Common Name:
Optical Structure Miscellaneo
Crystal (Symmetry Allowed): Non-
Atomic Coor
nd Harm.)

CIF (2θ, I pairs) (*.cif)
CIF (I, 10 per record) (*.cif)
ICDD Delimited text (*.csv)
ICDD Formatted text (*.prn)
ICDD XML (*.xml)



Inorganic Crystal Structural Database

Information center FIZ Karlsruhe

✓Inorganic Structures

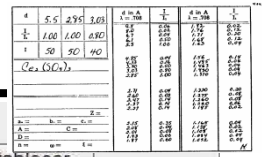
600 crystal structures elements
15000 records binary compounds
33000 records ternary compounds
35000 records quartenary compounds, etc..

- Structural data
- Atomic coordinates
- Bibliographic data
- Synthesis conditions

ICSD web
ICSD CD-ROM (FindIt)
ICSD intranet
ICSD Demo Version

ICSD Inorganic crystal structural database

http://icsd.iqfr.csic.es/icsd/



Authors/Code | Years | Journal | Title/Comment

Elements: Ce O | Element Count: 2 | Chem/Mineral Name | ANX/Pearson/S.Type

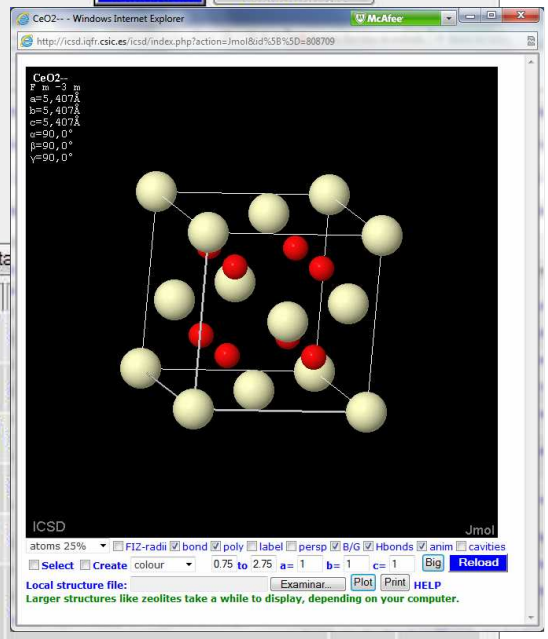
System: any | Laue Class: any | Centering: any | Space Group

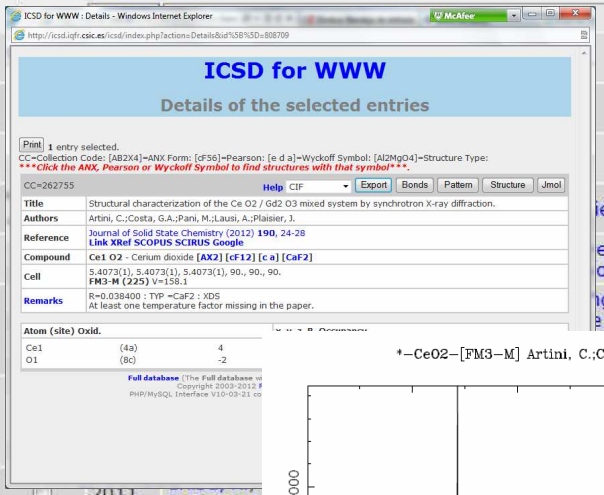
Remarks | Min. Distance | Distance Select | Distance Range

Help | Search | Restablecer

Query : (EL_COUNT = "2") AND icsd.sum_form RLIKE 'CE[0-9]' AND icsd.sum_form RLIKE BINARY 'O[0-9]'

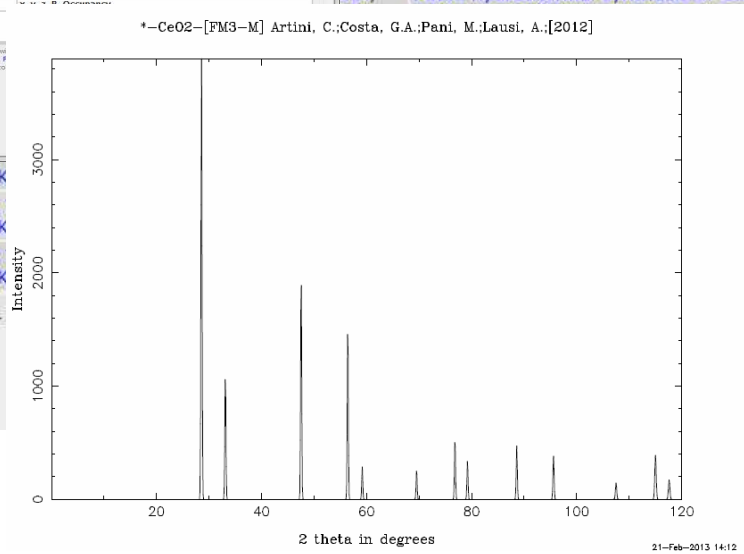
Select All / None 71 Results References EndNote Deta

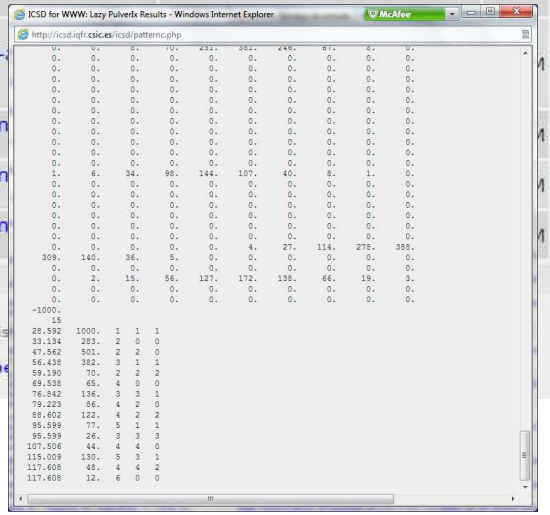




	Title
	Density functional calculations of the enthalpies of formation of rare-earth orthophosphates
	Density functional calculations of the enthalpies of formation of rare-earth orthophosphates
	Probing complex disorder in Ce1-x Gdx O2-x/2 using the pair distribution function analysis
ier, J.;	Structural characterization of the Ce O2 / Gd2 O3 mixed system by synchrotron X-ray diffraction
euk oo;	Dopant induced variations in microstructure and optical properties of Ce O2 nanoparticles
ng; e Di;	Facile hydrothermal synthesis of Ce O2 nanosheets with high reactive
2011 Nozawa, K	
2011 Chiba, R.; Nozawa, K	
2011 Chiba, R.; Nozawa, K	

Pages : [1] 2 3 4 5 6 7 8(71





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-x Prx O2-delta as an

-x Prx O2-delta as an

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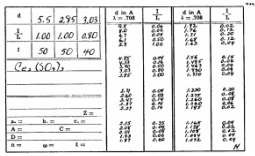
trum (FIZ) Karlsruhe

y Peter Hewat email: he

ICMAB

The Powder diffraction Database

CSIC



Cambridge Structural Database

Cambridge Crystallographic Data Center

✓small-molecule organic structures

✓metal-organic crystal structures

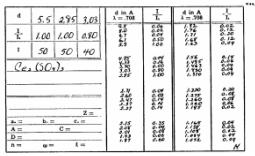
Containing the results of over half-a-million x-ray and neutron diffraction analyses

✓Chemical
✓Experimental
✓ Crystallographic
✓Bibliographic
✓Atomic coordinates

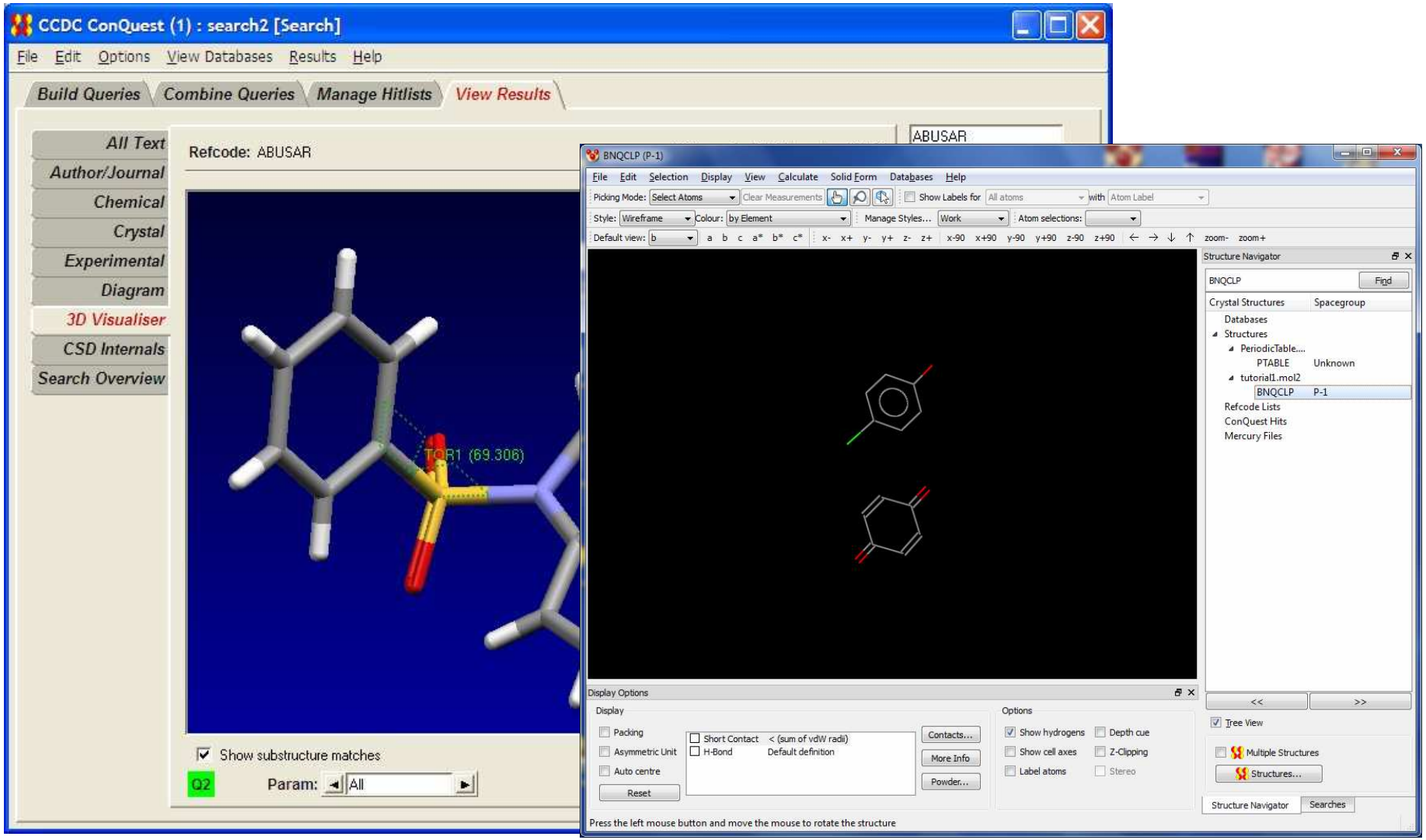
❖Software version
✓software for search and information retrieval(ConQuest)
✓structure visualisation (Mercury)
✓numerical analysis (Vista)
✓database creation (PreQuest)

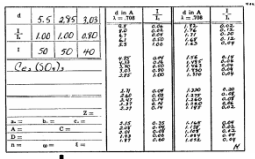
❖WebCSD

(Access requires personal registration)



http://www.xtal.iqfr.csic.es/data-bases/csd-spain.html





Crystal Data File

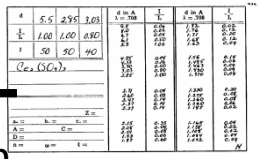
NIST- National Institute of Standards and Technology

✓Unit cell of crystalline materials

237000 entries

- ➢Standard cell parameters
- ➢Cell volume
- ➢Space group number and symbol
- ➢Chemical formula/name
- ➢Classification by chemical type

- ❖Is temporally UNAVAILABLE
- ❖(Is available in ICDD database)



Pauling File

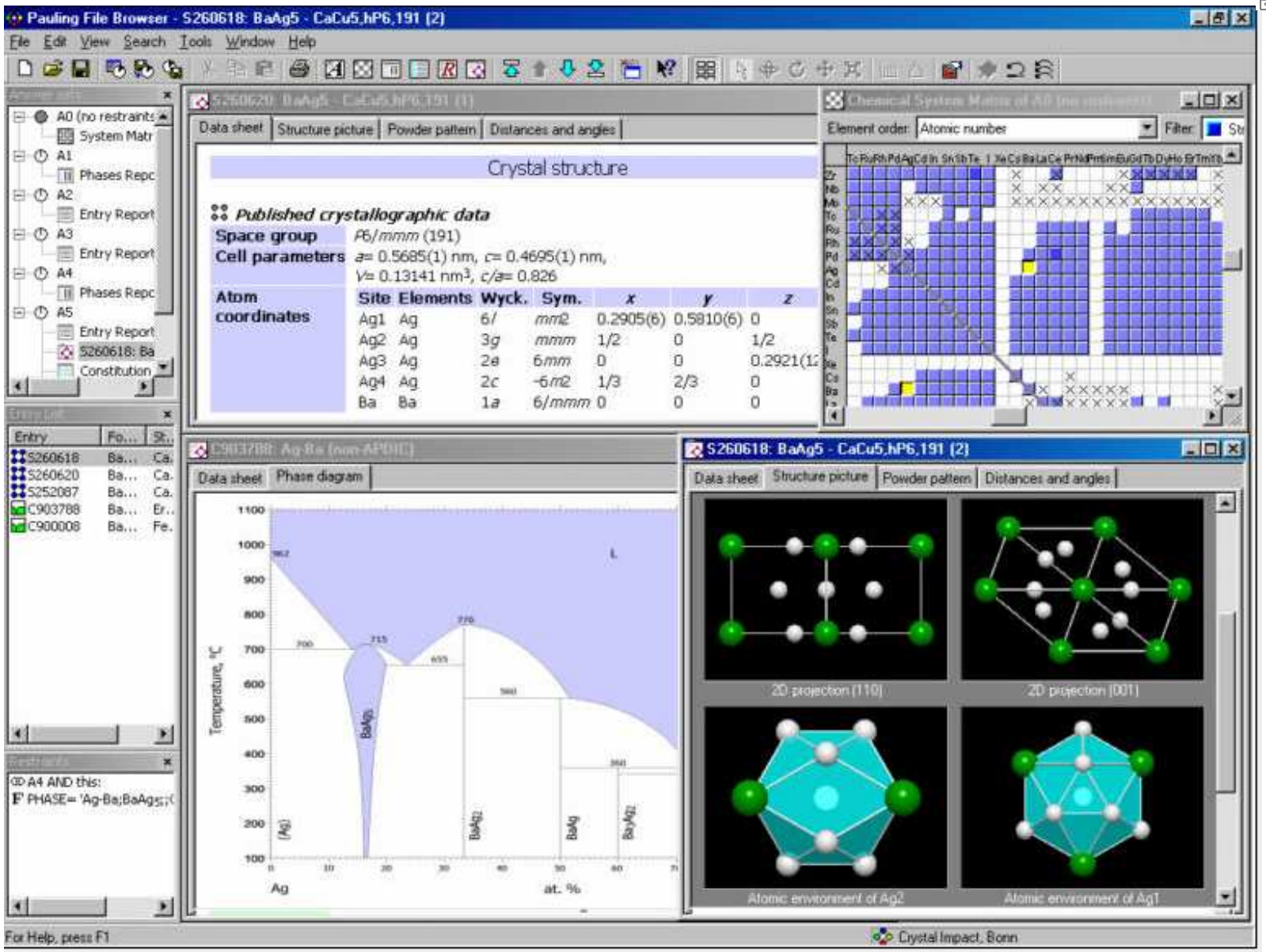
Japan Science and Technology Corporation
+
Material Phases Data System

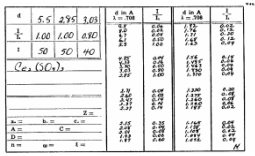
✓ Non-organic solid state materials

252599 Crystal structure entries
(38592Phase diagrams entries)
(91134 Physical property entries)

- Structure data
- Diffraction data
- Physical property data

- ❖Pauling Files Binaries Edition software
- ❖Pearson's Crystal Data software
- ❖PDF-4+ (ICDD)


Pauling File Browser - S260618: BaAg5 - CaCu5,hP6,191 (2)
File Edit View Search Tools Window Help
Data sheet
Structure picture
Powder pattern
Distances and angles
Crystal structure
Published crystallographic data
Space group
P6/mmm (191)
Cell parameters
a= 0.5685(1) nm, c= 0.4695(1) nm,
V= 0.13141 nm3, c/a= 0.826
Atom coordinates
Site Elements Wyck. Sym. x y z
Ag1 Ag 6/ mm2 0.2905(6) 0.5810(6) 0
Ag2 Ag 3g mmm 1/2 0 1/2
Ag3 Ag 2e 6mm 0 0 0.2921(12
Ag4 Ag 2c -6m2 1/3 2/3 0
Ba Ba 1a 6/mmm 0 0 0
Element order: Atomic number
Filter:
Data sheet
Phase diagram
Temperature, °C
at. %
Ag
S260618: BaAg5 - CaCu5,hP6,191 (2)
Data sheet
Structure picture
Powder pattern
Distances and angles
2D projection (110)
2D projection (001)
Atomic environment of Ag2
Atomic environment of Ag1
For Help, press F1
Crystal Impact, Bonn



CRYSTMET

Toth Information Systems

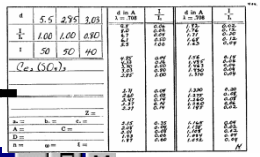
✓ crystallographic data for metals, including alloys, intermetallics and minerals

109,877 entries

- Crystallographic data
- Atomic coordinates
- Calculated powder diffraction patterns

❖Software

❖Trial version : Materials ToolKit Environment http://www.tothcanada.com/databases.htm



CRYSTMET(R) – The Metals Database

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Results

Periodic Table | Bibliographic | Unit Cell | Powder Patterns | Formula | ID Codes

	1A												3A	4A	5A	6A	7A	8A
1	H	2A																He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg	3B	4B	5B	6B	7B	8B			1B	2B	Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Rf	Ha													

Lanthanides	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Actinides	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Operator: (•) And ( ) Or ( ) Not

[✓] Require Coordinates [✓] Only selected elements

Query: element Cu

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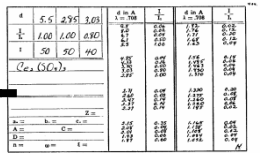


Protein data bank

Brookhaven National Laboratory

- ✓ Proteins
- ✓ Nucleic acids
- ✓ Other biological molecules

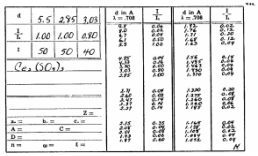
↓

8000 entries

↓

- ➢ Atomic coordinates
- ➢ Citations
- ➢ Structure information
- ➢ Crystallographic structure experimental data
- ➢ X-ray

- ❖ Available in CD-ROM
- ❖ Available web



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A MEMBER OF THE PDB | EMDataBank

An Information Portal to Biological Macromolecular Structures

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X-RAY DIFFRACTION

4EGC

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Materials and Methods page

Crystallization — Hide

Crystallization Experiments

Method	VAPOR DIFFUSION, HANGING DROP
pH	5.1
Temperature	291.0
Details	13.75% PEG8000, 0.01 M magnesium chloride, 0.05 M MES, pH 5.1, VAPOR DIFFUSION, HANGING DROP, temperature 291K

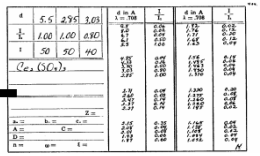
Crystal Data — Hide

Unit Cell

Length	(Å)	Angle	(°)
a =	123.21	**α** =	90
b =	150.18	**β** =	90
c =	53.92	**γ** =	90

Space Group

Space Group Name:	P 21 21 2



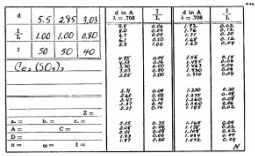
Mineralogy Database

✓ mineral species

4,714 entries

- crystal structures
- X-Ray powder diffraction
- chemical composition
- physical and optical properties
- Dana's New classification
- Strunz classification
- mineral specimen images
- alphabetical listings of mineral species

Web free access



X-Ray Diffraction Table

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Minerals Arranged by X-Ray Powder Diffraction

See Help on X-Ray Diffraction.

Powder X-ray Diffraction (XRD) is one of the primary techniques used by mineralogists and solid state chemists to examine the physico-chemical make-up of unknown materials. This data is represented in a collection of single-phase X-ray powder diffraction patterns for the three most intense D values in the form of tables of interplanar spacings (D), relative intensities (I/Io), mineral name and chemical formulae

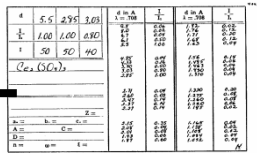
The XRD technique takes a sample of the material and places a powdered sample in a holder, then the sample is illuminated with x-rays of a fixed wave-length and the intensity of the reflected radiation is recorded using a goniometer. This data is then analyzed for the reflection angle to calculate the inter-atomic spacing (D value in Angstrom units - 10^{-8} cm). The intensity(I) is measured to discriminate (using I ratios) the various D spacings and the results are compared to this table to identify possible matches. Note: 2 theta (Θ) angle calculated from the Bragg Equation, $2\Theta = 2(\arcsin(n\lambda/(2d))$ where n=1;

For more information about this technique, see X-Ray Analysis of a Solid or take an internet course at Birkbeck College On-line Courses. Many thanks to Frederic Biret for these data.

Optional Search Query - To Reset, Click Here

Selected X-Ray λ	Change X-Ray λ	D_1 Å	D_2 Å	D_3 Å	Tolerance %	Elements	
1.54056 - CuKa1							Enviar consulta

[1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15] [16] [17] [18] [19] [20] [21] [22] [23] [24] [25] [26] [27] [28] [29] [30] [31] [32] [33] [34] [35] [36] [37] [38] [39] [40] [41] [42] [43] [44] [45] [46] [47] [48] [49] [50] [51] [52] [53] [54] [55] [56] [57] [58] [59] [60] [61] [62] [63] [64] [65]



Database of Zeolite Structures

International Zeolite Association (IZA)

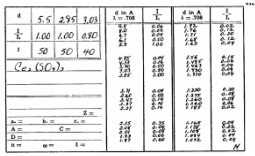
✓ Zeolite Framework Types

- descriptions and drawings of each framework type
- user-controlled animated displays of each framework type
- crystallographic data and simulated powder diffraction patterns
- relevant references
- detailed instructions for building model descriptions of some families of disordered zeolite structures

Web free access

Database of Zeolite Structures

http://www.iza-structure.org/databases/



Crystal data:

Composition: $[Si_{48}O_{96}]$

Refined composition: $[Si_{48}O_{96}]$

Space group: C1c1 (# 9) **Setting:**

Cell parameters: *a* = 18.524Å *b* = 5.0032Å *c* = 23.810Å
α = 90° β = 105.82° γ = 90°

Refinement: X-ray single crystal refinement, R_w=0.069

Reference: Dollase, W.A. and Baur, W.H.
Am. Mineral., **61**, 971-978 (1976)

Atomic Coordinates:

Atom	Form Factor	x	y	z	PP	B(iso)
Si1	Si	0.5507	0.541	0.5642	1.0	0.9
Si2	Si	0.7036	0.947	0.7374	1.0	1.2
Si3	Si	0.4198	0.549	0.6225	1.0	0.7
Si4	Si	0.5751	0.043	0.7955	1.0	1.1
Si5	Si	0.9247	0.548	0.6971	1.0	0.8
Si6	Si	0.7643	0.944	0.5386	1.0	0.9
Si7	Si	0.8023	0.449	0.7661	1.0	0.8
Si8	Si	0.6453	0.041	0.6027	1.0	0.7
Si9	Si	0.8531	0.463	0.9016	1.0	1.0
Si10	Si	0.9493	0.966	0.9358	1.0	1.0
Si11	Si	0.7244	0.559	0.9605	1.0	0.9
Si12	Si	0.5697	0.549	0.8702	1.0	1.1
O1	O	0.5749	0.351	0.8182	1.0	1.2
O2	O	0.5707	0.840	0.8476	1.0	1.5
O3	O	0.7315	0.138	0.4851	1.0	1.8
O4	O	0.7509	0.644	0.5152	1.0	1.7
O5	O	0.4155	0.352	0.6741	1.0	2.9
O6	O	0.4127	0.852	0.6434	1.0	1.9
O7	O	0.8773	0.164	0.9213	1.0	1.8
O8	O	0.9160	0.668	0.9361	1.0	2.4
O9	O	0.7741	0.145	0.7538	1.0	1.8
O10	O	0.7336	0.643	0.7402	1.0	2.2
O11	O	0.6195	0.341	0.5847	1.0	1.2
O12	O	0.5811	0.843	0.5661	1.0	1.9
O13	O	0.4966	0.511	0.6062	1.0	2.7
O14	O	0.3533	0.489	0.5665	1.0	1.0
O15	O	0.6498	0.005	0.6711	1.0	1.8
O16	O	0.6524	0.996	0.7805	1.0	2.0

Cell parameters: *a* = 18.524A *b* = 5.0032A *c* = 23.810Å
α = 90° β = 105.82° γ = 90°

eolite Structur
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Edit Data
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0.02 °2θ
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at °2θ
°2θ reflection (hkl)
Intensity axis: 0.0
er pattern
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HKL list:

h	k	l	2-Theta	d	I(rel)
0	0	2	7.712	11.4541	0.38
2	0	0	9.918	8.9112	0.20
-2	0	2	10.781	8.1996	0.00
2	0	2	14.147	6.2553	0.23
0	0	4	15.459	5.7270	0.05
-2	0	4	15.939	5.5557	0.04
1	1	0	18.403	4.8170	0.61
-1	1	1	18.526	4.7854	0.16
1	1	1	19.089	4.6455	0.00
-4	0	2	19.290	4.5975	2.39
-1	1	2	19.441	4.5621	1.06
4	0	0	19.911	4.4556	0.01
1	1	2	20.505	4.3278	100.00
2	0	4	20.577	4.3127	56.45
-1	1	3	21.051	4.2167	1.65
-4	0	4	21.658	4.0998	82.51
1	1	3	22.519	3.9450	0.34
-2	0	6	22.681	3.9173	0.59
-3	1	1	22.859	3.8871	1.27
-3	1	2	23.156	3.8379	0.07
-1	1	4	23.217	3.8280	27.05
3	1	0	23.224	3.8269	26.78
0	0	6	23.278	3.8180	15.71
4	0	2	23.292	3.8159	15.03
-3	1	3	24.093	3.6907	0.40
3	1	1	24.223	3.6712	3.06
1	1	4	24.996	3.5595	0.05
-3	1	4	25.603	3.4764	0.46
3	1	2	25.787	3.4520	2.49
-1	1	5	25.809	3.4491	2.30
-4	0	6	26.252	3.3919	4.50
-3	1	5	27.599	3.2293	3.50
2	0	6	27.793	3.2072	1.52
1	1	5	27.822	3.2040	1.32
3	1	3	27.827	3.2034	0.75
4	0	4	28.515	3.1276	0.92
-1	1	6	28.722	3.1056	0.00
-6	0	2	28.898	3.0870	1.10
-6	0	4	29.847	2.9911	0.11
-3	1	6	29.992	2.9769	6.09
-5	1	2	30.003	2.9758	7.32
-2	0	8	30.038	2.9724	4.48

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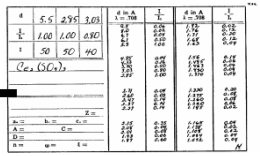

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- ✓ crystal structures of organic, inorganic, metal-organic compounds and minerals (excluding biopolymers)

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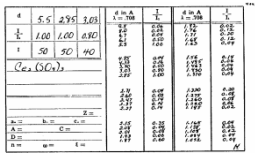

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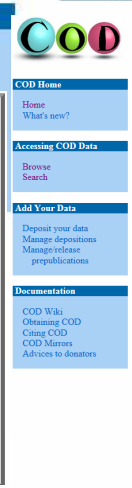
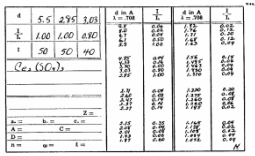


COD ID: 9007445
Formula: - Al4 O7 Sr -
Comments: Boyko, E. R.; Wisnyi, L. G. The optical properties and structures of CaO*2Al2O3 and SrO*2Al2O3 Locality: synthetic Acta Crystallographica 11 (1958) 444-445
Space group: C 1 2/c 1
Cell volume: 625.213
Cell parameters: 13.04; 9.01; 5.55; 90; 106.502; 90;

COD ID: 9007446
Formula: - Al4 Ca O7 -
Comments: Boyko, E. R.; Wisnyi, L. G. The optical properties and structures of CaO*2Al2O3 and SrO*2Al2O3 Locality: synthetic Acta Crystallographica 11 (1958) 444-445
Space group: C 1 2/c 1
Cell volume: 596.407
Cell parameters: 12.89; 8.88; 5.45; 90; 107.05; 90;

COD ID: 9007496
Formula: - Al2 O3 -
Comments: Lewis, J.; Schwarzenbach, D.; Flack, H. D. Electric field gradients and charge density in corundum alpha-Al2O3 Acta Crystallographica, Section A 38 (1982) 733-739
Space group: R -3 c :H
Cell volume: 254.977
Cell parameters: 4.7602; 4.7602; 12.9933; 90; 90; 120;

COD ID: 9007497
Formula: - Cu2 O -
Comments: Kirfel, A.; Eichhorn, K. Accurate structure analysis with synchrotron radiation. The electron density in Al2O3 and Cu2O Locality: synthetic Note: Atomic parameters were mislabeled in the publication. They have been fixed in this dataset. Acta Crystallographica, Section A 46 (1990) 271-284
Space group: P n -3 m :1
Cell volume: 77.772
Cell parameters: 4.2685; 4.2685; 4.2685; 90; 90; 90;

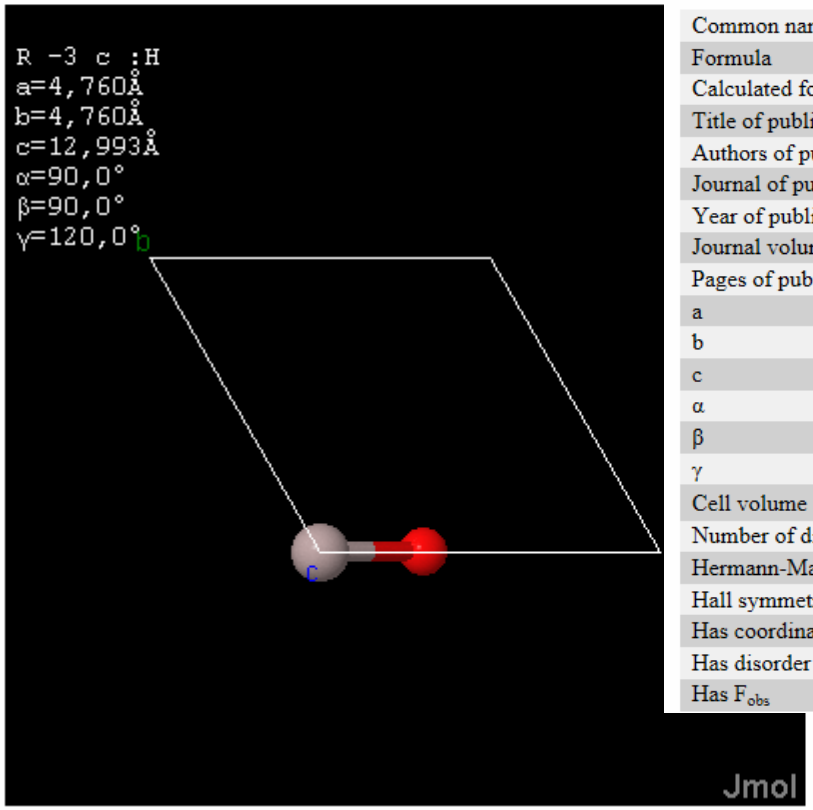


CIF Information Card

Information card for 9007496

9007495 << **9007496** >> 9007497

Preview



Structure parameters

Common name	Corundum
Formula	- Al2 O3 -
Calculated formula	- Al12 O18 -
Title of publication	Electric field gradients and charge density in corundum alpha-Al2O3
Authors of publication	Lewis, J.; Schwarzenbach, D.; Flack, H. D.
Journal of publication	Acta Crystallographica, Section A
Year of publication	1982
Journal volume	38
Pages of publication	733 - 739
a	4.7602 Å
b	4.7602 Å
c	12.9933 Å
α	90°
β	90°
γ	120°
Cell volume	254.977 $Å^3$
Number of distinct elements	2
Hermann-Mauguin symmetry space group	R -3 c :H
Hall symmetry space group	-R 3 2"c
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No