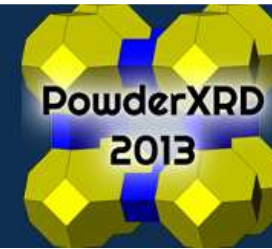




Data retrieval and Structure determination
from Synchrotron Powder Diffraction data
April 3-5 2013



The Powder Diffraction Database

Anna Crespi Revuelta

Servei General de Difracció de Raigs-X

Institut de Ciència de Materials de Barcelona

(acrespi@icmab.es)



4 April 2013



d	5.5	2.95	3.03	$\frac{1}{d}$	0.18	0.34	0.33	$\frac{1}{d}$	0.18	0.34	0.33
$\frac{1}{d}$	1.00	1.00	Δf_0	0.2	0.25	0.25	0.25	0.2	0.25	0.25	0.25
f	50	50	40	2.5	4.0	4.0	4.0	2.5	4.0	4.0	4.0
$(e_2, G(e_2))$				0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
				1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
				2.27	2.00	2.00	2.00	2.27	2.00	2.00	2.00
				2.30	0.00	0.00	0.00	2.30	0.00	0.00	0.00
				2.57	0.00	0.00	0.00	2.57	0.00	0.00	0.00
				2.57	0.00	0.00	0.00	2.57	0.00	0.00	0.00
				2.27	0.00	0.00	0.00	2.27	0.00	0.00	0.00
a_1, a_2				2.57	0.33	0.33	0.33	2.57	0.33	0.33	0.33
$A =$				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$B =$				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$D =$				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$g =$				1.57	0.50	0.50	0.50	1.57	0.50	0.50	0.50

What's a powder diffraction database?

The Powder Diffraction File

Databases and search-match programs

Powder Diffraction File Database


Exemples PDF-4+

- Search Filters (3)
- Sieve+ Program (1)
- Export atomic coordinates (1)

3. OTHER SPECIFIC DATABASES



4	5.5	2.95	3.03	$\frac{1}{2} \ln A$	$\frac{1}{2}$	$\frac{1}{2} \ln A$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.70	0.70	0.7
				1.0	1.00	1.00	1.0
$(\rho_{\text{ex}}(G))_i$				1.5	0.85	0.85	0.8
				2.0	0.80	0.80	0.7
				2.5	0.75	0.75	0.6
				3.0	0.70	0.70	0.5
				3.5	0.65	0.65	0.4
				4.0	0.60	0.60	0.3
				4.5	0.55	0.55	0.2
				5.0	0.50	0.50	0.1
				5.5	0.45	0.45	0.0
				6.0	0.40	0.40	0.0
				6.5	0.35	0.35	0.0
				7.0	0.30	0.30	0.0
				7.5	0.25	0.25	0.0
				8.0	0.20	0.20	0.0
				8.5	0.15	0.15	0.0
				9.0	0.10	0.10	0.0
				9.5	0.05	0.05	0.0
				10.0	0.00	0.00	0.0



The figure shows an X-ray diffraction (XRD) pattern for a crystal. The vertical axis is labeled I (Intensity) and the horizontal axis is labeled 2θ (diffraction angle). The pattern displays several sharp, well-defined diffraction peaks, indicating a high degree of crystallinity. The word "Crystal" is written in the upper right area of the plot.



ICSD

ICDD®
INTERNATIONAL CENTER FOR DIFFRACTION DATA

RCB PDB
PROTEIN DATA BANK

33-1161		d \bar{A}	Int	hk ℓ	d \bar{A}	Int	hk
SiO ₂		4.257	22	100	1.1532	1	311
Silicon Oxide		3.342	100	101	1.1405	<1	204
Quartz, syn		2.457	8	110	1.1143	<1	303
		2.282	8	102	1.0813	2	312
Rad. CuK α_1	λ 1.540598 Filter Mono.	2.237	4	111	1.0635	<1	400
Cut off	Int. Diffractometer						
Ref. Natl. Bur. Stand. (U.S.) Monogr. 25, 18 61 (1981)	d-sp Diff. l/l_{cor} 3.6	2.127	6	200	1.0476	1	105
		1.9792	4	201	1.0438	<1	401
Sys. Hexagonal	S.G. P3 ₂ 1 (154)	1.8179	14	112	1.0347	<1	214
a 4.9133(2) b	c 5.4053(4) A C 1.1001	1.8021	<1	003	1.0150	1	223
α β	γ Z 3 mp	1.6719	4	202	0.9898	1	402
Ref. Ibid.		1.6591	2	103	0.9873	1	313
D _x 2.65	D _m 2.66 SS/FOM F ₃₀ = 77.(013,31)	1.6082	<1	210	0.9783	<1	304
$e\alpha$	$no\beta$ 1.544 $e\gamma$ 1.553 Sign +2V	1.5418	9	211	0.9762	1	320
Ref. Swanson, Fuyat, Natl. Bur. Stand. (U.S.), Circ. 539, 3 24 (1954)		1.4536	1	113	0.9636	<1	205
		1.4189	<1	300			
Color Colorless		1.3820	6	212			
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 ₂ Si 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.		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			

d	5.5	2.95	3.03	d in A	1	d in A	1
$\frac{1}{d}$	1.00	1.00	AYO	0.2	0.25	1.12	0.12
t	50	50	40	0.3	0.35	1.17	0.12
$\rho_{e, G(\rho_e)}$				0.4	0.45	1.21	0.12
				0.5	0.55	1.25	0.12
				0.6	0.65	1.29	0.12
				0.7	0.75	1.33	0.12
				0.8	0.85	1.37	0.12
				0.9	0.95	1.41	0.12
				1.0	1.00	1.45	0.12
				1.1	1.10	1.49	0.12
				1.2	1.20	1.53	0.12
				1.3	1.30	1.57	0.12
				1.4	1.40	1.61	0.12
				1.5	1.50	1.65	0.12
				1.6	1.60	1.69	0.12
				1.7	1.70	1.73	0.12
				1.8	1.80	1.77	0.12
				1.9	1.90	1.81	0.12
				2.0	2.00	1.85	0.12
				2.1	2.10	1.89	0.12
				2.2	2.20	1.93	0.12
				2.3	2.30	1.97	0.12
				2.4	2.40	2.01	0.12
				2.5	2.50	2.05	0.12
				2.6	2.60	2.09	0.12
				2.7	2.70	2.13	0.12
				2.8	2.80	2.17	0.12
				2.9	2.90	2.21	0.12
				3.0	3.00	2.25	0.12
				3.1	3.10	2.29	0.12
				3.2	3.20	2.33	0.12
				3.3	3.30	2.37	0.12
				3.4	3.40	2.41	0.12
				3.5	3.50	2.45	0.12
				3.6	3.60	2.49	0.12
				3.7	3.70	2.53	0.12
				3.8	3.80	2.57	0.12
				3.9	3.90	2.61	0.12
				4.0	4.00	2.65	0.12
				4.1	4.10	2.69	0.12
				4.2	4.20	2.73	0.12
				4.3	4.30	2.77	0.12
				4.4	4.40	2.81	0.12
				4.5	4.50	2.85	0.12
				4.6	4.60	2.89	0.12
				4.7	4.70	2.93	0.12
				4.8	4.80	2.97	0.12
				4.9	4.90	3.01	0.12
				5.0	5.00	3.05	0.12
				5.1	5.10	3.09	0.12
				5.2	5.20	3.13	0.12
				5.3	5.30	3.17	0.12
				5.4	5.40	3.21	0.12
				5.5	5.50	3.25	0.12
				5.6	5.60	3.29	0.12
				5.7	5.70	3.33	0.12
				5.8	5.80	3.37	0.12
				5.9	5.90	3.41	0.12
				6.0	6.00	3.45	0.12
				6.1	6.10	3.49	0.12
				6.2	6.20	3.53	0.12
				6.3	6.30	3.57	0.12
				6.4	6.40	3.61	0.12
				6.5	6.50	3.65	0.12
				6.6	6.60	3.69	0.12
				6.7	6.70	3.73	0.12
				6.8	6.80	3.77	0.12
				6.9	6.90	3.81	0.12
				7.0	7.00	3.85	0.12
				7.1	7.10	3.89	0

X-ray Röntgen

Bragg's law

X-ray diffraction

1978 *International Centre for Diffraction Data*



The Powder diffraction Database



INTRODUCTION: Past and Present

d	h	k	l	d	h	k	l
5.5	2.95	1.01	1.01	5.5	2.95	1.01	1.01
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
50	50	50	50	50	50	50	50
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							
$Ce_2(SiO_4)_2$							

Primary refere

00-046-1045

Sep 5, 2012 10:11 AM (jgil)

Status Primary QM: Star (S) Pressure/Temperature: Ambient Chemical Formula: SiO2

Empirical Formula: O2 Si Weight %: O53.26 Si46.74 Atomic %: O66.67 Si33.33

Compound Name: Silicon Oxide Mineral Name: Quartz, syn

Radiation: CuK α 1 λ : 1.5406Å Filter: Ge Mono d-Spacing: Diff. Intensity: Diffractometer Illic: 3.41

SYS: Hexagonal SPGR: P3221 (154)

Author's Cell [AuthCell a: 4.9134Å AuthCell b: 4.9134Å AuthCell c: 5.40524(8)Å AuthCell Vol: 113.01Å³ AuthCell Z: 3.00

AuthCell MolVol: 37.67 [AuthCell's Cell Axial Ratio [cla: 1.100] Dealo: 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 [XtiCell a: 4.913Å XtiCell b: 4.913Å XtiCell c: 5.405Å XtiCell α : 90.00° XtiCell β : 90.00°

XtiCell γ : 120.00° XtiCell Vol: 113.01Å³ XtiCell Z: 3.00]

Crystal Data Axial Ratio [cla: 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]

μ = 1.544 ϵ = 1.553 Sign: ==

Crystal (Symmetry Allowed): Centrosymmetric

Pearson: hP9.00 Prototype Structure: SiO2 Prototype Structure (Alpha Order): O2 Si

LPF Prototype Structure: SiO2.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. 198, 177 (1992).

Additional Patterns: To replace 00-033-1161. See PDF 01-085-0335. Color: White. General
Database Comments: Comments: Low temperature quartz, 28 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 K α 1 1.54056Å

2 θ	d(Å)	I	h	k	l	*	2 θ	d(Å)	I	h	k	l	*	2 θ	d(Å)	I	h	k	l	*
20.8595	4.254990	16	1	0	0		77.8730	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		114.8347	0.915176	2	4	1	1	
39.4841	2.281490	8	1	0	2		81.1707	1.183980	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	8	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		87.4368	1.114550	<1	3	0	3		121.8479	0.881352	<1	1	0	6	
50.6208	1.801740	<1	0	0	3		90.8284	1.081550	2	3	1	2		122.5996	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	1.452880	2	1	1	3		98.7472	1.014900	1	2	2	3		136.4169	0.829680	1	2	0	6	
65.7842	1.418410	<1	3	0	0		102.2275	0.989578	<1	1	1	5		137.8875	0.825393	2	4	1	3	
67.7421	1.382100	8	2	1	2		102.5835	0.987248	<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	
68.3181	1.371880	5	3	0	1		104.1994	0.976174	<1	3	2	0		144.1101	0.809688	<1	3	3	1	
73.4858	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								

Int	hkl
14	

Mar 7, 2013 1:19 PM (jgil)

Pressure/Temperature: Ambient Chemical Formula: Ce2 (S O4)3
t %: Ce49.30 O33.78 Si6.92 Atomic %: Ce11.76 O70.59 Si17.65

acing: D.S. Camera Diameter: 406.40

Dmeas: 3.912g/cm³

[XtiCell 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
ial Research Council Bulletin 107. Decomposition temperature is 920 C at 746
source: Powder Diffraction.

ensity) - Cu K α 1 1.54056Å

d(Å)	I	h	k	l	*	2 θ	d(Å)	I	h	k	l	*
22.270000	14					65.1846	1.430000	4				
75.215000	35					68.4228	1.370000	4				
16.208000	4					71.4006	1.320000	20				
70.201000	8					73.9952	1.280000	8				
50.193000	6					75.3719	1.260000	8				
03.187000	60					78.3036	1.220000	6				
75.820000	2					80.6758	1.190000	2				
92.176000	12					82.3497	1.170000	4				
59.171000	20					85.0146	1.140000	2				
07.168000	12					87.8866	1.110000	2				
18.163000	4					89.9307	1.090000	4				
72.156000	14					94.3781	1.050000	4				
54.146000	4											

1941



The Powder diffraction Database



[illegible]

Sep 5, 2012 10:11 AM (jail)

Compound Name: Silicon Oxide Mineral Name: Quartz, syn

Radiation: CuK α 1 λ : 1.5406Å Filter: Ge Mono d-Spacing: Diff. Intensity: Diffractometer Illc: 3.41SSIFOM: $F(30) = 558.3(0.0017, 31)$

RedCell β : 90.00° RedCell γ : 120.00° RedCell Vol: 113.01 Å³

$\pi\omega\beta$: =1.544 ϵ_V : =1.553 Sign: =+

Crystal (Symmetry Allowed): Centrosymmetric

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. 198, 177 (1992).

Additional Patterns: To replace 00-033-1161. See PDF 01-085-0335. Color: White. General

Database Comments: Comments: Low temperature quartz. 2θ determination based on profile fit method. Temperature of Data Collection: Pattern taken at 295(1) K. Unit Cell Data Source: Powder Diffraction.

d-Spacings (5 θ) - 00-046-1045 (Fixed Slit Intensity) - Cu K α 1.54056Å

20	d(Å)	I	h	k	l	*	20	d(Å)	I	h	k	l	*	20	d(Å)	I	h	k	l	*
20.8595	4.254990	16	1	0	0		77.8730	1.228320	1	2	2	0		114.0566	0.918159	<1	3	2	2	
26.6393	3.434470	100	1	0	1		79.8817	1.199820	2	2	1	3		114.4825	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		115.8808	0.908890	<1	2	2	4	
40.2989	2.236130	4	1	0	1		81.4888	1.180170	2	3	1	0		117.5323	0.900685	<1	0	2	6	
42.7919	2.127710	6	2	0	0		83.8377	1.140850	<1	3	3	1		118.3081	0.897188	<1	2	1	5	
45.7918	1.979680	4	2	0	1		84.9548	1.140850	<1	2	0	4		120.1191	0.888910	1	3	1	4	
50.1375	1.817960	13	1	1	2		87.4368	1.114550	<1	3	0	3		121.8479	0.881352	<1	1	0	6	
50.6206	1.801740	<1	0	0	3		90.8284	1.061550	2	3	1	2		122.5998	0.878187	<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	0.845937	<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	0.825960	1	2	0	6	
65.7842	1.418410	<1	3	0	0		102.2275	0.989576	<1	1	1	5		137.9875	0.825393	2	4	1	3	
67.7421	1.392100	6	2	1	2		102.5635	0.987246	<1	3	1	3		140.3102	0.818911	<1	3	3	0	
68.1730	1.374030	7	3	0	1		103.8733	0.983833	<1	3	0	3		143.2434	0.811682	3	3	3	2	
68.3161	1.371880	5	3	0	1		104.1994	0.976174	<1	3	2	0		144.1101	0.809668	<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	0.928526	<1	4	1	0								

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

d	$h^2 + k^2 + l^2$	h	k	l	d	$h^2 + k^2 + l^2$	h	k	l
5.5	275	13	13	13	5.5	275	13	13	13
1.00	100	10	0	0	1.00	100	10	0	0
50	50	7	7	0	50	50	7	7	0
(Ca ₂ SiO ₄) ₂									

d	$h^2 + k^2 + l^2$	h	k	l
1.00	1.00	1.00	0.00	0.00
0.71	1.00	0.71	0.00	0.00
0.50	1.00	0.50	0.00	0.00
0.35	1.00	0.35	0.00	0.00
0.29	1.00	0.29	0.00	0.00
0.25	1.00	0.25	0.00	0.00
0.22	1.00	0.22	0.00	0.00
0.20	1.00	0.20	0.00	0.00
0.18	1.00	0.18	0.00	0.00
0.16	1.00	0.16	0.00	0.00
0.14	1.00	0.14	0.00	0.00
0.12	1.00	0.12	0.00	0.00
0.11	1.00	0.11	0.00	0.00
0.10	1.00	0.10	0.00	0.00
0.09	1.00	0.09	0.00	0.00
0.08	1.00	0.08	0.00	0.00
0.07	1.00	0.07	0.00	0.00
0.06	1.00	0.06	0.00	0.00
0.05	1.00	0.05	0.00	0.00
0.04	1.00	0.04	0.00	0.00
0.03	1.00	0.03	0.00	0.00
0.02	1.00	0.02	0.00	0.00
0.01	1.00	0.01	0.00	0.00

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

☐ Not

ICDD (00) Or

ICSD-FIZ (01)

Cambridge (02)

NIST (03)

LPF (04)

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) Or

Rietveld (R)

Indexed (I)

Calculated (C)

Blank (B)

Low-Precision (O)

Prototyping (P)

Hypothetical (H)

Good (G)

Minimal Acceptable (M)

Subfile/Subclass

☐ Not

Intermetallics

Ionic Conductors

Merck

Metals & Alloys

Micro & Mesoporous

Mineral Related

Modulated Structure

NBS

Nucleosides & Nucleotides

Organics

Pharmaceutical

Pigment

Polymer

Porphyryns, Corrins & Complexes

Steroids

Superconducting Material

Terpenes

Thermoelectric Material

Search Show Results Undock Page Reset Page Reset All

4	5.5	2.95	3.03	$\frac{1}{2} \ln A$	$\frac{1}{2}$	$\frac{1}{2} \ln A$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.70	0.70	0.7
				0.8	0.80	0.80	0.8
				0.9	0.90	0.90	0.9
				1.0	1.00	1.00	1.0
				1.1	1.10	1.10	1.1
				1.2	1.20	1.20	1.2
				1.3	1.30	1.30	1.3
				1.4	1.40	1.40	1.4
				1.5	1.50	1.50	1.5
				1.6	1.60	1.60	1.6
				1.7	1.70	1.70	1.7
				1.8	1.80	1.80	1.8
				1.9	1.90	1.90	1.9
				2.0	2.00	2.00	2.0
				2.1	2.10	2.10	2.1
				2.2	2.20	2.20	2.2
				2.3	2.30	2.30	2.3
				2.4	2.40	2.40	2.4
				2.5	2.50	2.50	2.5
				2.6	2.60	2.60	2.6
				2.7	2.70	2.70	2.7
				2.8	2.80	2.80	2.8
				2.9	2.90	2.90	2.9
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				3.2	3.20	3.20	3.2
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				3.4	3.40	3.40	3.4
				3.5	3.50	3.50	3.5
				3.6	3.60	3.60	3.6
				3.7	3.70	3.70	3.7
				3.8	3.80	3.80	3.8
				3.9	3.90	3.90	3.9
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				4.3	4.30	4.30	4.3
				4.4	4.40	4.40	4.4
				4.5	4.50	4.50	4.5
				4.6	4.60	4.60	4.6
				4.7	4.70	4.70	4.7
				4.8	4.80	4.80	4.8
				4.9	4.90	4.90	4.9
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				5.2	5.20	5.20	5.2
				5.3	5.30	5.30	5.3
				5.4	5.40	5.40	5.4
				5.5	5.50	5.50	5.5
				5.6	5.60	5.60	5.6
				5.7	5.70	5.70	5.7
				5.8	5.80	5.80	5.8
				5.9	5.90	5.90	5.9
				6.0	6.00	6.00	6.0
				6.1	6.10	6.10	6.1
				6.2	6.20	6.20	6.2
				6.3	6.30	6.30	6.3
				6.4	6.40	6.40	6.4
				6.5	6.50	6.50	6.5
				6.6	6.60	6.60	6.6
				6.7	6.70	6.70	6.7
				6.8	6.80	6.80	6.8
				6.9	6.90	6.90	6.9
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				7.1	7.10	7.10	7.1
				7.2	7.20	7.20	7.2
				7.3	7.30	7.30	7.3
				7.4	7.40	7.40	7.4
				7.5	7.50	7.50	7.5
				7.6	7.60	7.60	7.6
				7.7	7.70	7.70	7.7
				7.8	7.80	7.80	7.8
				7.9	7.90	7.90	7.9
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				8.1	8.10	8.10	8.1
				8.2	8.20	8.20	8.2
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				8.4	8.40	8.40	8.4
				8.5	8.50	8.50	8.5
				8.6	8.60	8.60	8.6
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				8.8	8.80	8.80	8.8
				8.9	8.90	8.90	8.9
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				9.2	9.20	9.20	9.2
				9.3	9.30	9.30	9.3
				9.4	9.40	9.40	9.4
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				9.6	9.60	9.60	9.6
				9.7	9.70	9.70	9.7
				9.8	9.80	9.80	9.8
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				10.3	10.30	10.30	10.3
				10.4	10.40	10.40	10.4
				10.5	10.50	10.50	10.5
				10.6	10.60	10.60	10.6
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				11.1	11.10	11.10	11.1
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				11.3	11.30	11.30	11.3
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				11.6	11.60	11.60	11.6
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				11.9	11.90	11.90	11.9
				12.0	12.00	12.00	12.0
				12.1	12.10	12.10	12.1
				12.2	12.20	12.20	12.2
				12.3	12.30	12.30	12.3
				12.4	12.40	12.40	12.4
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				13.1	13.10	13.10	13.1
				13.2	13.20	13.20	13.2
				13.3	13.30	13.30	13.3
				13.4	13.40	13.40	13.4
				13.5	13.50	13.50	13.5
				13.6	13.60	13.60	13.6
				13.7	13.70	13.70	13.7
				13.8	13.80	13.80	13.8
				13.9	13.90	13.90	13.9
				14.0	14.00	14.00	14.0
				14.1	14.10	14.10	14.1
				14.2	14.20	14.20	14.2
				14.3	14.30	14.30	14.3
				14.4	14.40	14.40	14.4
				14.5	14.50	14.50	14.5
				14.6	14.60	14.60	14.6
				14.7	14.70	14.70	14.7
				14.8	14.80	14.80	14.8
				14.9	14.90	14.90	14.9
				15.0	15.00	15.00	15.0
				15.1	15.10	15.10	15.1
				15.2	15.20	15.20	15.2
				15.3	15.30	15.30	15.3
				15.4	15.40	15.40	15.4
				15.5	15.50	15.50	15.5
				15.6	15.60	15.60	15.6
				15.7	15.70	15.70	15.7
				15.8	15.80	15.80	15.8
				15.9	15.90	15.90	15.9
				16.0	16.00	16.00	16.0
				16.1	16.10	16.10	16.1
				16.2	16.20	16.20	16.2
				16.3	16.30	16.30	16.3
				16.4	16.40	16.40	16.4
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				16.8	16.80	16.80	16.8
				16.9	16.90	16.90	16.9
				17.0	17.00	17.00	17.0
				17.1	17.10	17.10	17.1
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				17.6	17.60	17.60	17.6
				17.7	17.70	17.70	17.7
				17.8	17.80	17.80	17.8
				17.9	17.90	17.90	17.9
				18.0	18.00	18.00	18.0
				18.1	18.10	18.10	18.1
				18.2	18.20	18.20	18.2
				18.3	18.30	18.30	18.3
				18.4	18.40	18.40	18.4
				18.5	18.50	18.50	18.5
				18.6	18.60	18.60	18.6
				18.7	18.70	18.70	18.7
				18.8	18.80	18.80	18.8
				18.9	18.90	18.90	18.9
				19.0	19.00	19.00	19.0
				19.1	19.10	19.10	19.1
				19.2	19.20	19.20	19.2
				19.3	19.30	19.30	19.3
				19.4	19.40	19.40	19.4
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				19.6	19.60	19.60	19.6
				19.7	19.70	19.70	19.7
				19.8	19.80	19.80	19.8
				19.9	19.90	19.90	19.9
				20.0	20.00	20.00	20.0
				20.1	20.10	20.10	20.1
				20.2	20.20	20.20	20.2
				20.3	20.30	20.30	20.3
				20.4	20.40	20.40	20.4
				20.5	20.50	20.50	20.5
				20.6	20.60	20.60	20.6
				20.7	20.70	20.70	20.7
				20.8	20.80	20.80	20.8
				20.9	20.90	20.90	20.9
				21.0	21.00	21.00	21.0
				21.1	21.10	21.10	21.1
				21.2	21.20	21.20	21.2
				21.3	21.30	21.30	21.3
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				21.6	21.60	21.60	21.6
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				22.0	22.00	22.00	22.0
				22.1	22.10	22.10	22.1
				22.2	22.20	22.20	22.2
				22.3	22.30		

Search

Global Operator

Numeric Input

Help

Subfiles/Database Filters

Periodic Table

Elements

Names

References

Structures

Miscellaneous

Compound Name

☐ Not

Contains Words

Common Name

☐ Not

Contains Words

Mineral Name

☐ Not

Contains Words

All Names

☐ Not

Contains Words

Zeolite Classification

☐ Not

ABW - Li-A(BW)
 ACO - ACP-1
 AEI - AlPO4-18
 AEL - AlPO4-11
 AEN - AlPO-EN3
 AET - AlPO4-8
 AFG - Afghanistan
 AFI - AlPO4-5
 AFN - AlPO-14
 AFO - AlPO4-41
 AFR - SAPO-40
 AFS - MAPSO-46
 AFT - AlPO4-52
 AFX - SAPO-56
 AGL - AlPO-18

Mineral Classification






☐ Not

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 - Ancyrite (Supergroup)
 ADA - Andalusite (Group)
 ANT - Antlerite (Group)
 APA - Apatite (Group)
 APH - Aphthitalite (Supergroup)
 APC - Anophyllite (Supergroup)

Structure: Please select a class

Results - {Compound Name Contains Wo...

File Edit Fields Results Similarity Index Help

Results (2 of 328,660)

Search Preference Set: ▼

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

h	5.5	2.75	1.03	h'	1	h''	1	h'''	1
k	1.00	1.00	0.50	k'	1	k''	1	k'''	1
l	50	50	50	l'	1	l''	1	l'''	1
Cu ₂ (O ₂ C ₆ H ₄) ₂									
a	1.382	1.382	1.382	a'	1.382	a''	1.382	a'''	1.382
b	1.382	1.382	1.382	b'	1.382	b''	1.382	b'''	1.382
c	1.382	1.382	1.382	c'	1.382	c''	1.382	c'''	1.382
α	90	90	90	α'	90	α''	90	α'''	90
β	90	90	90	β'	90	β''	90	β'''	90
γ	90	90	90	γ'	90	γ''	90	γ'''	90

C13 H18 O2 - 00-032-1723

File Edit d-Spacings Tools Window Help

2D

d-Spacings

Wavelength: Cu Kα1 1.54056 Å

Stick Patterns

☒ Fixed Slit Intensity
☐ Variable Slit Intensity
☐ Integrated Intensity

Diffraction Patterns

☒ Simulated Profile
☐ Raw Diffraction Data (PD3)

2θ	d(Å)	I	h	k	l	*
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	

Intensity

00

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:

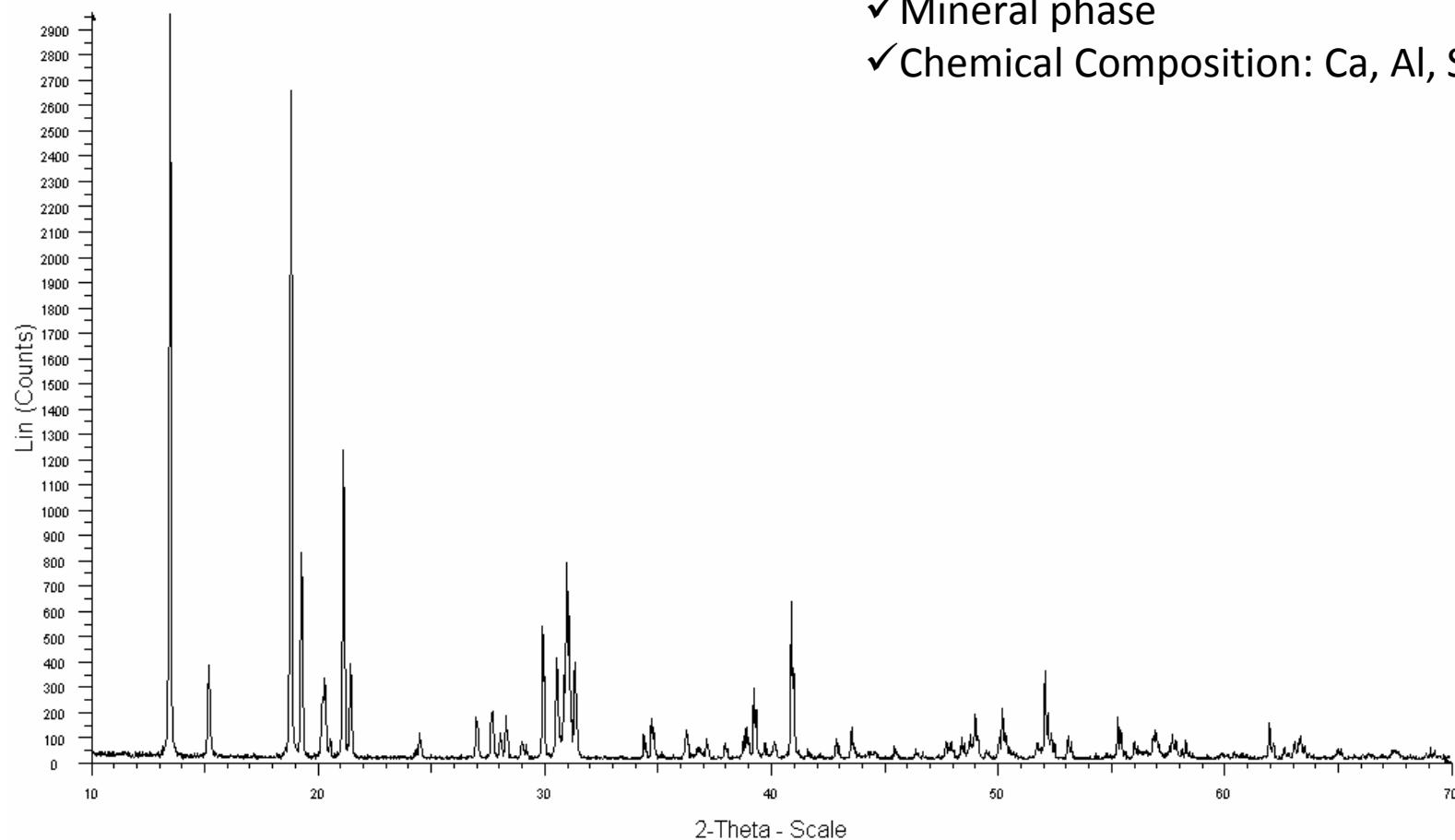
Compound Name: Ibuprofen

Mineral Name:

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

d	5.5	2.95	3.03	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$
$\frac{1}{\lambda}$	1.00	1.00	0.90	0.2	0.000	0.15	0.000
l	50	50	40	0.3	0.000	0.17	0.000
				0.4	0.000	0.18	0.000
				0.5	0.000	0.19	0.000
				0.6	0.000	0.20	0.000
				0.7	0.000	0.21	0.000
				0.8	0.000	0.22	0.000
				0.9	0.000	0.23	0.000
				1.0	0.000	0.24	0.000
				1.1	0.000	0.25	0.000
				1.2	0.000	0.26	0.000
				1.3	0.000	0.27	0.000
				1.4	0.000	0.28	0.000
				1.5	0.000	0.29	0.000
				1.6	0.000	0.30	0.000
				1.7	0.000	0.31	0.000
				1.8	0.000	0.32	0.000
				1.9	0.000	0.33	0.000
				2.0	0.000	0.34	0.000
				2.1	0.000	0.35	0.000
				2.2	0.000	0.36	0.000
				2.3	0.000	0.37	0.000
				2.4	0.000	0.38	0.000
				2.5	0.000	0.39	0.000
				2.6	0.000	0.40	0.000
				2.7	0.000	0.41	0.000
				2.8	0.000	0.42	0.000
				2.9	0.000	0.43	0.000
				3.0	0.000	0.44	0.000
				3.1	0.000	0.45	0.000
				3.2	0.000	0.46	0.000
				3.3	0.000	0.47	0.000
				3.4	0.000	0.48	0.000
				3.5	0.000	0.49	0.000
				3.6	0.000	0.50	0.000
				3.7	0.000	0.51	0.000
				3.8	0.000	0.52	0.000
				3.9	0.000	0.53	0.000
				4.0	0.000	0.54	0.000
				4.1	0.000	0.55	0.000
				4.2	0.000	0.56	0.000
				4.3	0.000	0.57	0.000
				4.4	0.000	0.58	0.000
				4.5	0.000	0.59	0.000
				4.6	0.000	0.60	0.000
				4.7	0.000	0.61	0.000
				4.8	0.000	0.62	0.000
				4.9	0.000	0.63	0.000
				5.0	0.000	0.64	0.000
				5.1	0.000	0.65	0.000
				5.2	0.000	0.66	0.000
				5.3	0.000	0.67	0.000
				5.4	0.000	0.68	0.000
				5.5	0.000	0.69	0.000
				5.6	0.000	0.70	0.000
				5.7	0.000	0.71	0.000
				5.8	0.000	0.72	0.000
				5.9	0.000	0.73	0.000

Example 2



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

SCOLECITE - File: SCOLECITE.raw - Type: 2Th/Th locked - Start: 10.000 ° - End: 70.000 ° - Step: 0.020 ° - Step time: 1. s - Creation: 26/11/2002 14:34:07
Operations: Import



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d	5.5	2.95	3.03	d in A 1 in B	$\frac{1}{d}$	d in A 1 in B	$\frac{1}{d}$
$\frac{1}{d}$	1.00	1.00	0.90	0.9	2.22	1.12	0.91
1	50	50	40	4.7	0.17	1.17	0.86
				2.3	0.43	1.25	0.80
Ces. 60.00				0.95	0.95	1.05	0.95
				1.22	0.82	1.05	0.95
				1.22	0.82	1.10	0.91
				2.3	0.43	1.30	0.77
				2.47	0.40	1.30	0.77
				2.57	0.39	1.37	0.73
				2.57	0.39	1.47	0.68
				2.57	0.39	1.57	0.64
				2.57	0.39	1.67	0.60
				2.57	0.39	1.77	0.57
				2.57	0.39	1.87	0.53
				2.57	0.39	1.97	0.51
				2.57	0.39	2.07	0.48
				2.57	0.39	2.17	0.46
				2.57	0.39	2.27	0.44
				2.57	0.39	2.37	0.42
				2.57	0.39	2.47	0.40
				2.57	0.39	2.57	0.39
				2.57	0.39	2.67	0.37
				2.57	0.39	2.77	0.36
				2.57	0.39	2.87	0.34
				2.57	0.39	2.97	0.33
				2.57	0.39	3.07	0.32
				2.57	0.39	3.17	0.31
				2.57	0.39	3.27	0.30
				2.57	0.39	3.37	0.29
				2.57	0.39	3.47	0.28
				2.57	0.39	3.57	0.28
				2.57	0.39	3.67	0.27
				2.57	0.39	3.77	0.26
				2.57	0.39	3.87	0.26
				2.57	0.39	3.97	0.25
				2.57	0.39	4.07	0.24
				2.57	0.39	4.17	0.24
				2.57	0.39	4.27	0.23
				2.57	0.39	4.37	0.23
				2.57	0.39	4.47	0.22
				2.57	0.39	4.57	0.22
				2.57	0.39	4.67	0.21
				2.57	0.39	4.77	0.21
				2.57	0.39	4.87	0.20
				2.57	0.39	4.97	0.20
				2.57	0.39	5.07	0.20
				2.57	0.39	5.17	0.19
				2.57	0.39	5.27	0.19
				2.57	0.39	5.37	0.18
				2.57	0.39	5.47	0.18
				2.57	0.39	5.57	0.18
				2.57	0.39	5.67	0.17
				2.57	0.39	5.77	0.17
				2.57	0.39	5.87	0.17
				2.57	0.39	5.97	0.16
				2.57	0.39	6.07	0.16
				2.57	0.39	6.17	0.16
				2.57	0.39	6.27	0.15
				2.57	0.39	6.37	0.15

[illegible]

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)

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)

Subfile/Subclass

☐ Not

- Ionic Conductors
- Merck
- Metals & Alloys
- Micro & Mesoporous
- Mineral Related
 - No Subclass
 - Mineral
 - Gem
 - Natural
 - Synthetic
- Modulated Structure
- NBS
- Nucleosides & Nucleotides
- Organics
- Pharmaceutical
- Pigment
- Polymer

Search Show Results Unlock Page Reset Page Reset All

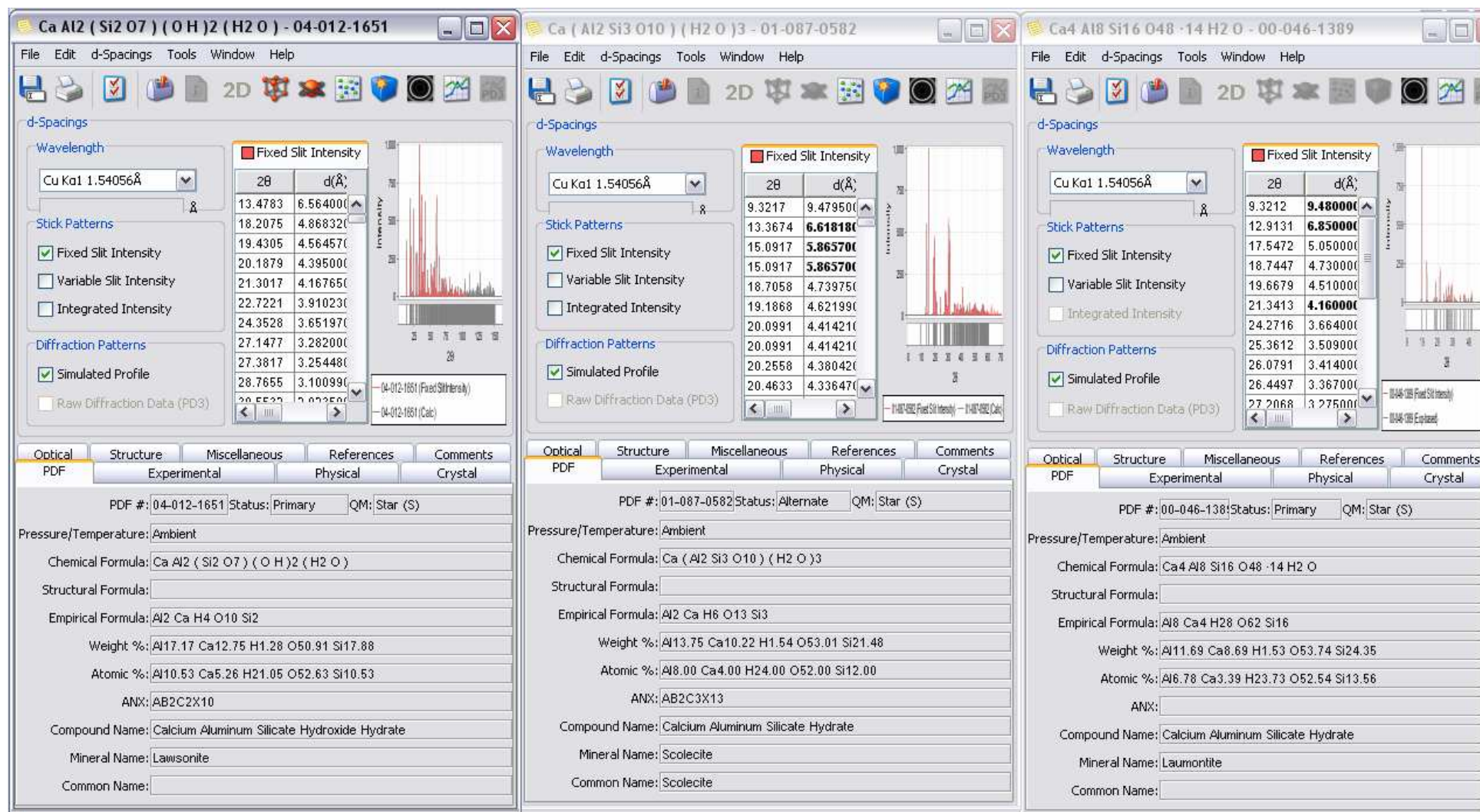
Results - [Quality Map (Star (S))] ...											
File Edit Fields Results Similarity Index Help											
Results (14 of 329,660)											
Search Preference Set: ICDD Defaults											
PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1	D2	D3	SYS	AuthCell a	AuthCell b	
00-034-0137	S	Ca ₂ A ₄ S ₁₈ O ₂₄ H ₂ O	Calcium Aluminum Silicate Hydrate	Chabazite-Ca	4.323000	2.927000	9.340000	R	13.784	-	-
00-039-1381	S	Ca ₂ (Si ₈ A ₃)O ₂₄ H ₂ O	Calcium Aluminum Silicate Hydrate	Epistilbite	8.900000	3.446000	3.208000	M	9.089	17.747	-
00-042-1451	S	Ca ₂ Al ₂ Si ₄ O ₁₂ H ₂ O	Calcium Aluminum Silicate Hydrate	Wairakite	3.386000	5.560000	3.409000	M	13.6947	13.6377	-
00-046-1389	S	Ca ₄ A ₈ S ₁₆ O ₄₈ H ₂ O	Calcium Aluminum Silicate Hydrate	Laumontite	9.480000	6.850000	4.160000	M	14.77	13.09	-
00-047-1785	S	Ca ₄ A ₈ S ₁₆ O ₄₈ H ₂ O	Calcium Aluminum Silicate Hydrate	Laumontite	9.440000	4.152000	6.840000	M	14.747	13.075	-
01-087-0582	S	Ca ₂ (A ₂ Si ₃ O ₁₀) ₂ (H ₂ O) ₃	Calcium Aluminum Silicate Hydrate	Scolecite	5.865700	2.887390	6.618180	M	18.489	18.959	-
04-012-1651	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.721350	2.629690	2.619510	O	5.847	8.79	-
04-012-1652	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.723160	2.631680	2.622010	O	5.851	8.799	-
04-012-1653	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.726080	2.634660	2.625170	O	5.857	8.81	-
04-012-1685	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.721770	2.630180	2.621620	O	8.797	5.852	-
04-012-1686	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.720770	2.629450	2.623920	O	8.789	5.843	-
04-012-1687	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.701830	2.610040	2.598340	O	8.717	5.805	-
04-012-1688	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.736120	2.644810	2.637420	O	8.852	5.882	-
04-012-1689	S	Ca ₂ (Al ₂ Si ₂ O ₇)(OH) ₂ (H ₂ O)	Calcium Aluminum Silicate Hydroxide...	Lawsoneite	2.737960	2.646570	2.639870	O	8.86	5.888	-



The Powder diffraction Database

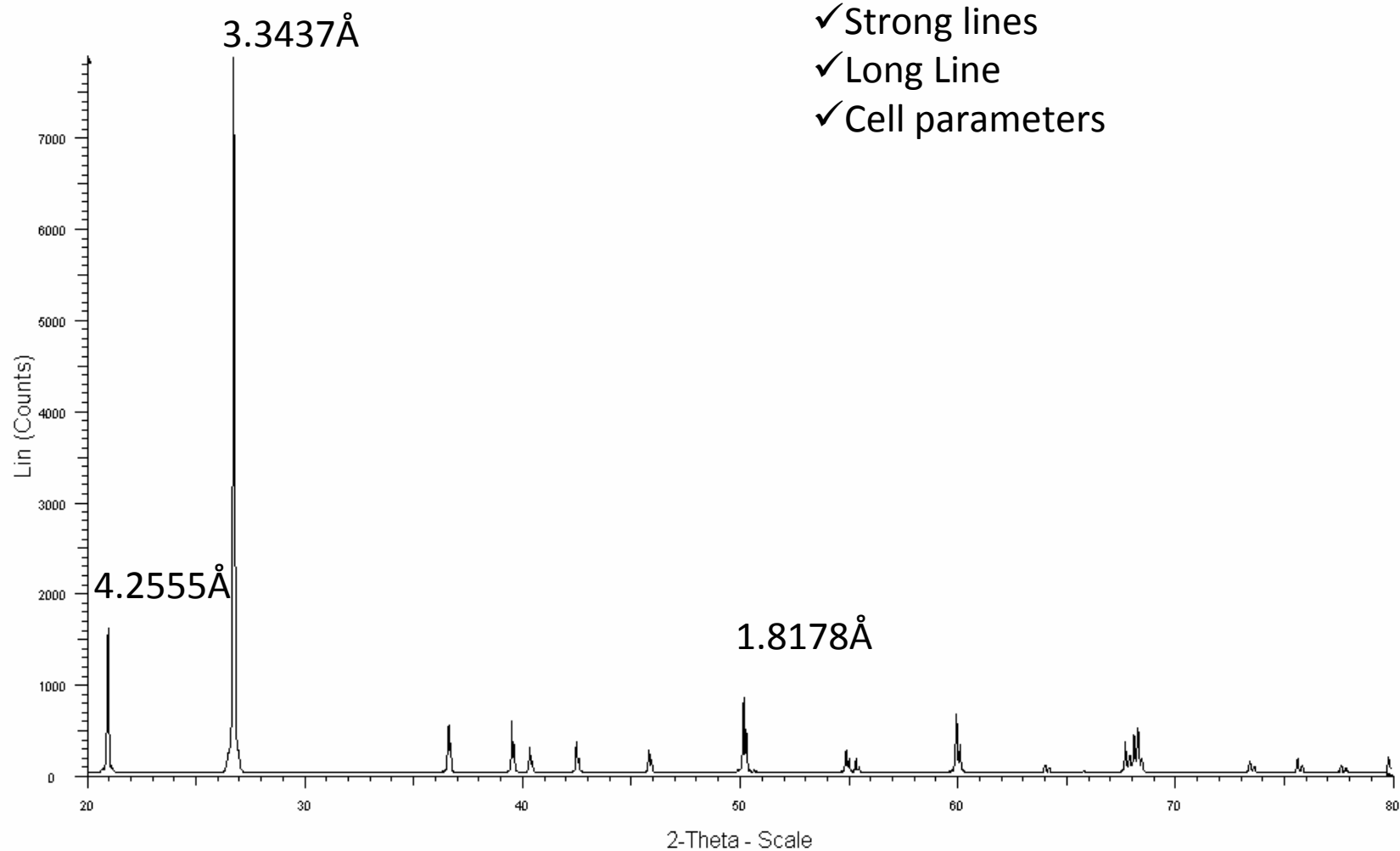


4	5.5	2.95	3.03	$\frac{1}{2} \ln A$	$\frac{1}{2}$	$\frac{1}{2} \ln A$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.70	0.70	0.7
				0.8	0.80	0.80	0.8
				0.9	0.90	0.90	0.9
				1.0	1.00	1.00	1.0
				1.1	1.10	1.10	1.1
				1.2	1.20	1.20	1.2
				1.3	1.30	1.30	1.3
				1.4	1.40	1.40	1.4
				1.5	1.50	1.50	1.5
				1.6	1.60	1.60	1.6
				1.7	1.70	1.70	1.7
				1.8	1.80	1.80	1.8
				1.9	1.90	1.90	1.9
				2.0	2.00	2.00	2.0
				2.1	2.10	2.10	2.1
				2.2	2.20	2.20	2.2
				2.3	2.30	2.30	2.3
				2.4	2.40	2.40	2.4
				2.5	2.50	2.50	2.5
				2.6	2.60	2.60	2.6
				2.7	2.70	2.70	2.7
				2.8	2.80	2.80	2.8
				2.9	2.90	2.90	2.9
				3.0	3.00	3.00	3.0
				3.1	3.10	3.10	3.1
				3.2	3.20	3.20	3.2
				3.3	3.30	3.30	3.3
				3.4	3.40	3.40	3.4
				3.5	3.50	3.50	3.5
				3.6	3.60	3.60	3.6
				3.7	3.70	3.70	3.7
				3.8	3.80	3.80	3.8
				3.9	3.90	3.90	3.9
				4.0	4.00	4.00	4.0
				4.1	4.10	4.10	4.1
				4.2	4.20	4.20	4.2
				4.3	4.30	4.30	4.3
				4.4	4.40	4.40	4.4
				4.5	4.50	4.50	4.5
				4.6	4.60	4.60	4.6
				4.7	4.70	4.70	4.7
				4.8	4.80	4.80	4.8
				4.9	4.90	4.90	4.9
				5.0	5.00	5.00	5.0
				5.1	5.10	5.10	5.1
				5.2	5.20	5.20	5.2
				5.3	5.30	5.30	5.3
				5.4	5.40	5.40	5.4
				5.5	5.50	5.50	5.5
				5.6	5.60	5.60	5.6
				5.7	5.70	5.70	5.7
				5.8	5.80	5.80	5.8
				5.9	5.90	5.90	5.9
				6.0	6.00	6.00	6.0
				6.1	6.10	6.10	6.1
				6.2	6.20	6.20	6.2
				6.3	6.30	6.30	6.3
				6.4	6.40	6.40	6.4
				6.5	6.50	6.50	6.5
				6.6	6.60	6.60	6.6
				6.7	6.70	6.70	6.7
				6.8	6.80	6.80	6.8
				6.9	6.90	6.90	6.9
				7.0	7.00	7.00	7.0
				7.1	7.10	7.10	7.1
				7.2	7.20	7.20	7.2
				7.3	7.30	7.30	7.3
				7.4	7.40	7.40	7.4
				7.5	7.50	7.50	7.5
				7.6	7.60	7.60	7.6
				7.7	7.70	7.70	7.7
				7.8	7.80	7.80	7.8
				7.9	7.90	7.90	7.9
				8.0	8.00	8.00	8.0
				8.1	8.10	8.10	8.1
				8.2	8.20	8.20	8.2
				8.3	8.30	8.30	8.3
				8.4	8.40	8.40	8.4
				8.5	8.50	8.50	8.5
				8.6	8.60	8.60	8.6
				8.7	8.70	8.70	8.7
				8.8	8.80	8.80	8.8
				8.9	8.90	8.90	8.9
				9.0	9.00	9.00	9.0
				9.1	9.10	9.10	9.1
				9.2	9.20	9.20	9.2
				9.3	9.30	9.30	9.3
				9.4	9.40	9.40	9.4
				9.5	9.50	9.50	9.5
				9.6	9.60	9.60	9.6
				9.7	9.70	9.70	9.7
				9.8	9.80	9.80	9.8
				9.9	9.90	9.90	9.9
				10.0	10.00	10.00	10.0
				10.1	10.10	10.10	10.1
				10.2	10.20	10.20	10.2
				10.3	10.30	10.30	10.3
				10.4	10.40	10.40	10.4
				10.5	10.50	10.50	10.5
				10.6	10.60	10.60	10.6
				10.7	10.70	10.70	10.7
				10.8	10.80	10.80	10.8
				10.9	10.90	10.90	10.9
				11.0	11.00	11.00	11.0
				11.1	11.10	11.10	11.1
				11.2	11.20	11.20	11.2
				11.3	11.30	11.30	11.3
				11.4	11.40	11.40	11.4
				11.5	11.50	11.50	11.5
				11.6	11.60	11.60	11.6
				11.7	11.70	11.70	11.7
				11.8	11.80	11.80	11.8
				11.9	11.90	11.90	11.9
				12.0	12.00	12.00	12.0
				12.1	12.10	12.10	12.1
				12.2	12.20	12.20	12.2
				12.3	12.30	12.30	12.3
				12.4	12.40	12.40	12.4
				12.5	12.50	12.50	12.5
				12.6	12.60	12.60	12.6
				12.7	12.70	12.70	12.7
				12.8	12.80	12.80	12.8
				12.9	12.90	12.90	12.9
				13.0	13.00	13.00	13.0
				13.1	13.10	13.10	13.1
				13.2	13.20	13.20	13.2
				13.3	13.30	13.30	13.3
				13.4	13.40	13.40	13.4
				13.5	13.50	13.50	13.5
				13.6	13.60	13.60	13.6
				13.7	13.70	13.70	13.7
				13.8	13.80	13.80	13.8
				13.9	13.90	13.90	13.9
				14.0	14.00	14.00	14.0
				14.1	14.10	14.10	14.1
				14.2	14.20	14.20	14.2
				14.3	14.30	14.30	14.3
				14.4	14.40	14.40	14.4
				14.5	14.50	14.50	14.5
				14.6	14.60	14.60	14.6
				14.7	14.70	14.70	14.7
				14.8	14.80	14.80	14.8
				14.9	14.90	14.90	14.9
				15.0	15.00	15.00	15.0
				15.1	15.10	15.10	15.1
				15.2	15.20	15.20	15.2
				15.3	15.30	15.30	15.3
				15.4	15.40	15.40	15.4
				15.5	15.50	15.50	15.5
				15.6	15.60	15.60	15.6
				15.7	15.70	15.70	15.7
				15.8	15.80	15.80	15.8
				15.9	15.90	15.90	15.9
				16.0	16.00	16.00	16.0
				16.1	16.10	16.10	16.1
				16.2	16.20	16.20	16.2
				16.3	16.30	16.30	16.3
				16.4	16.40	16.40	16.4
				16.5	16.50	16.50	16.5
				16.6	16.60	16.60	16.6
				16.7	16.70	16.70	16.7
				16.8	16.80	16.80	16.8
				16.9	16.90	16.90	16.9
				17.0	17.00	17.00	17.0
				17.1	17.10	17.10	17.1
				17.2	17.20	17.20	17.2
				17.3	17.30	17.30	17.3
				17.4	17.40	17.40	17.4
				17.5	17.50	17.50	17.5
				17.6	17.60	17.60	17.6
				17.7	17.70	17.70	17.7
				17.8	17.80	17.80	17.8
				17.9	17.90	17.90	17.9
				18.0	18.00	18.00	18.0
				18.1	18.10	18.10	18.1
				18.2	18.20	18.20	18.2
				18.3	18.30	18.30	18.3
				18.4	18.40	18.40	18.4
				18.5	18.50	18.50	18.5
				18.6	18.60	18.60	18.6
				18.7	18.70	18.70	18.7
				18.8	18.80	18.80	18.8
				18.9	18.90	18.90	18.9
				19.0	19.00	19.00	19.0
				19.1	19.10	19.10	19.1
				19.2	19.20	19.20	19.2
				19.3	19.30	19.30	19.3
				19.4	19.40	19.40	19.4
				19.5	19.50	19.50	19.5
				19.6	19.60	19.60	19.6
				19.7	19.70	19.70	19.7
				19.8	19.80	19.80	19.8
				19.9	19.90	19.90	19.9
				20.0	20.00	20.00	20.0
				20.1	20.10	20.10	20.1
				20.2	20.20	20.20	20.2
				20.3	20.30	20.30	20.3
				20.4	20.40	20.40	20.4
				20.5	20.50	20.50	20.5
				20.6	20.60	20.60	20.6
				20.7	20.70	20.70	20.7
				20.8	20.80	20.80	20.8
				20.9	20.90	20.90	20.9
				21.0	21.00	21.00	21.0
				21.1	21.10	21.10	21.1
				21.2	21.20	21.20	21.2
				21.3	21.30	21.30	21.3
				21.4	21.40	21.40	21.4
				21.5	21.50	21.50	21.5
				21.6	21.60	21.60	21.6
				21.7	21.70	21.70	21.7
				21.8	21.80	21.80	21.8
				21.9	21.90	21.90	21.9
				22.0	22.00	22.00	22.0
				22.1	22.10	22.10	22.1
				22.2	22.20	22.20	22.2
				22.3	22.30		



4	5.5	2.95	3.03	$\frac{1}{2} \ln A$	$\frac{1}{2}$	$\frac{1}{2} \ln A$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.57	0.77	0.7
				1.0	1.00	1.00	1.0
$(\rho_{\text{ex}}(G))_i$				1.5	0.69	1.15	0.6
				2.0	0.77	1.34	0.7
				2.5	0.80	1.47	0.8
				3.0	0.83	1.57	0.9
				3.5	0.85	1.65	0.9
				4.0	0.86	1.70	1.0
				4.5	0.87	1.74	1.0
				5.0	0.88	1.77	1.0
				5.5	0.88	1.79	1.0
				6.0	0.89	1.81	1.0
				6.5	0.89	1.82	1.0
				7.0	0.90	1.83	1.0
				7.5	0.90	1.84	1.0
				8.0	0.90	1.85	1.0
				8.5	0.90	1.85	1.0
				9.0	0.90	1.86	1.0
				9.5	0.90	1.86	1.0
				10.0	0.90	1.86	1.0
				10.5	0.90	1.86	1.0
				11.0	0.90	1.86	1.0
				11.5	0.90	1.86	1.0
				12.0	0.90	1.86	1.0
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				26.0	0.90	1.86	1.0
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				47.0	0.90	1.86	1.0
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				62.5	0.90	1.86	1.0
				63.0	0.90	1.86	1.0
				63.5	0.90	1.86	1.0
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				64.5	0.90	1.86	1.0
				65.0	0.90	1.86	1.0
				65.5	0.90	1.86	1.0
				66.0	0.90	1.86	1.0
				66.5	0.90	1.86	1.0
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				98.0	0.90	1.86	1.0
				98.5	0.90	1.86	1.0
				99.0	0.90	1.86	1.0
				99.5	0.90	1.86	1.0
				100.0	0.90	1.86	1.0

Example 3



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

4	5.5	2.95	3.03	$\frac{1}{2} \ln \frac{A}{B}$	$\frac{1}{2}$	$\frac{1}{2} \ln \frac{A}{B}$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.70	0.70	0.7
				1.0	1.00	1.00	1.0
$(\rho_{\text{ex}}(G))_i$				1.5	0.85	0.85	0.85
				2.0	0.80	0.80	0.80
				2.5	0.75	0.75	0.75
				3.0	0.70	0.70	0.70
				3.5	0.65	0.65	0.65
				4.0	0.60	0.60	0.60
				4.5	0.55	0.55	0.55
				5.0	0.50	0.50	0.50
				5.5	0.45	0.45	0.45
				6.0	0.40	0.40	0.40
				6.5	0.35	0.35	0.35
				7.0	0.30	0.30	0.30
				7.5	0.25	0.25	0.25
				8.0	0.20	0.20	0.20
				8.5	0.15	0.15	0.15
				9.0	0.10	0.10	0.10
				9.5	0.05	0.05	0.05
				10.0	0.00	0.00	0.00


The screenshot displays the CambridgeSoft Search application window. At the top, there is a 'Search' title bar and a menu bar with 'Global Operator', 'Numeric Input', and 'Help'. Below the menu bar is a tabbed interface with tabs for 'Subfiles/Database Filters', 'Periodic Table', 'Elements', 'Names', 'References', 'Structures', and 'Miscellaneous'. The 'Miscellaneous' tab is currently selected.

The main search area is divided into several sections, each with a blue header and a light gray background:

- Long Line:** Contains a search criterion: ☐ Not 4.2555 Å ESD: 0.3 Å. To the right, there is a vertical list of labels: L1, L2, L3.
- Strong Line:** Contains a search criterion: ☐ Not 3.3437 Å ESD: 0.3 Å. To the right, there is a vertical list of labels: D1, D2, D3.
- I/I-cc:** Contains a search criterion: ☐ Not 4.2555 Å ESD: 0.3 Å. To the right, there is a vertical list of labels: D1, D2, D3.
- Melting Point:** Contains a search criterion: ☐ Not [] ESD: [] °C °K °F. To the right, there is a vertical list of labels: Dcalc, Dstruc.
- Color:** Contains a search criterion: ☐ Not [] And [] Or []. The color list includes: Black, Blue, Brown, Color Missing, Colorless, Gray, Green.
- R-factor:** Contains a search criterion: ☐ Not 1.8178 Å ESD: 0.3 Å. To the right, there is a vertical list of labels: D1, D2, D3.
- Organic F:** Contains a search criterion: ☐ 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). To the right, there is a vertical list of labels: D1, D2, D3.
- Smith-Snyder Figure Of Merit (SS/FOM):** Contains a search criterion: ☐ Not [] ESD: [].
- Has PD3 Pattern:** Contains a search criterion: ☐ Yes ☐ No.
- Has Property Sheet:** Contains a search criterion: ☐ Yes ☐ No.
- Database Comments:** Contains a search criterion: ☐ Not Contains Words [] [].


At the bottom of the window, there is a row of buttons: 'Search', 'Show Results', 'Undock Page', 'Reset Page', and 'Reset All'.

h	5.5	2.95	3.03	h	1	1	1	h	1	1	1	h	1	1	1
k	1.00	1.00	1.00	k	1	1	1	k	1	1	1	k	1	1	1
l	50	50	50	l	1	1	1	l	1	1	1	l	1	1	1
C ₂ Cl ₂															


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

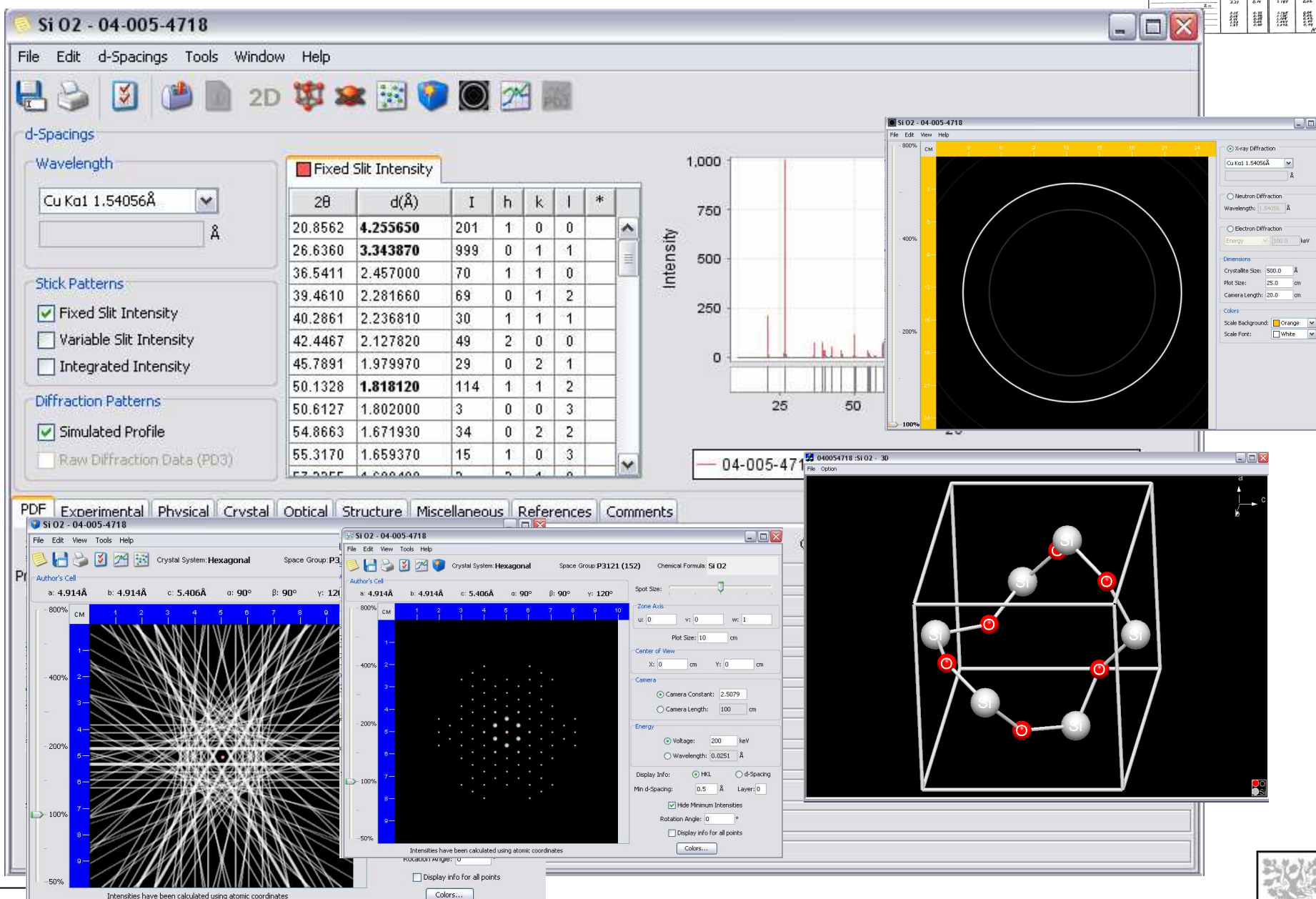
PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1	D2	D3	SYS	AuthCell a	AuthCell b	AuthCell c	AuthCell α	AuthCell β	AuthCell
01-085-0865	I	Si O ₂	Silicon Oxide	Quartz, syn	3.336560	4.243520	1.814370	H	4.9		5.4			
01-085-0930	S	Si O ₂	Silicon Oxide	Quartz, syn	3.342840	4.253050	1.817670	H	4.911		5.407			
01-085-1053	I	Si O ₂	Silicon Oxide	Quartz, syn	3.342940	4.254610	1.817610	H	4.9128		5.4042			
01-085-1054	S	Si O ₂	Silicon Oxide	Quartz	3.343530	4.255390	1.817930	H	4.9137		5.4051			
01-086-1560	S	Si O ₂	Silicon Oxide	Quartz	3.344560	4.257380	1.818440	H	4.916		5.4054			
01-086-1628	S	Si O ₂	Silicon Oxide	Quartz, syn	3.337370	4.245340	1.814750	H	4.9021		5.3997			
01-086-1629	S	Si O ₂	Silicon Oxide	Quartz, syn	3.337800	4.246120	1.814970	H	4.903		5.3999			
01-086-1630	S	Si O ₂	Silicon Oxide	Quartz, syn	3.343910	4.255740	1.818140	H	4.9141		5.406			
01-086-2237	I	Si O ₂	Silicon Oxide	Quartz	3.342970	4.254780	1.817620	H	4.913		5.404			
01-087-2096	S	Si O ₂	Silicon Oxide	Quartz low, syn	3.342960	4.254520	1.817630	H	4.9127		5.4045			
01-088-2487	H	Si O ₂	Silicon Oxide	Quartz, syn	3.345560	4.269510	1.818140	H	4.93		5.385			
01-089-1961	I	Si O ₂	Silicon Oxide	Quartz low, syn	3.349170	4.261710	1.821060	H	4.921		5.416			
01-089-8934	S	Si O ₂	Silicon Oxide	Quartz	3.343430	4.255390	1.817870	H	4.9137		5.4047			
01-089-8935	S	Si O ₂	Silicon Oxide		3.347500	4.261620	1.819990	H	4.9209		5.4091			
01-089-8936	S	Si O ₂	Silicon Oxide		3.352610	4.269250	1.822690	H	4.9297		5.4151			
01-089-8937	S	Si O ₂	Silicon Oxide		3.357730	4.276780	1.825390	H	4.9384		5.4213			
01-089-8938	S	Si O ₂	Silicon Oxide		3.364680	4.287610	1.829020	H	4.9509		5.4285			
01-089-8939	S	Si O ₂	Silicon Oxide		3.371450	4.297910	1.832560	H	4.9628		5.436			
03-065-0466	I	O ₂ Si	Silicon Oxide	Quartz low, syn	3.343910	4.255740	1.818140	H	4.9141		5.406			
04-001-9367	P	Si O ₂	Silicon Oxide		3.340770	4.252180	1.816400	H	4.91		5.4			
04-002-3600	P	Si O ₂	Silicon Oxide	Quartz	3.343280	4.255130	1.817790	H	4.9134		5.4046			
04-003-6495	P	Si O ₂	Silicon Oxide	Quartz	3.343450	4.254780	1.817920	H	4.913		5.406			
04-005-4494	B	Si O ₂	Silicon Oxide	Quartz, syn	3.342680	4.254250	1.817470	H	4.9124		5.4039			
04-005-4718	S	Si O ₂	Silicon Oxide	Quartz, syn	3.343870	4.255650	1.818120	H	4.914		5.406			
04-006-1767	P	Si O ₂	Silicon Oxide	Quartz	3.337820	4.246120	1.814980	H	4.903		5.4			
04-006-5050	P	Si O ₂	Silicon Oxide		3.343000	4.254700	1.817640	H	4.9129		5.4043			
04-007-5142	P	Si O ₂	Silicon Oxide	quartz	3.343270	4.254960	1.817790	H	4.9132		5.4049			
04-007-9911	P	Si O ₂	Silicon Oxide	quartz low	3.342470	4.254180	1.817340	H	4.9123		5.4031			
04-008-2359	P	Si O ₂	Silicon Oxide	quartz low	3.342940	4.254520	1.817620	H	4.9127		5.4044			
04-008-4810	I	Ge _{0.14} Si _{0.86} O ₂	Germanium Silicon Oxide	Quartz, germanian, syn	3.372230	4.294620	1.833330	H	4.959		5.446			
04-008-7651	I	Si O ₂	Silicon Oxide	Quartz	3.344250	4.256340	1.818320	H	4.9148		5.4062			
04-008-7652	I	Si O ₂	Silicon Oxide	quartz low	3.344280	4.256260	1.818340	H	4.9147		5.4065			
04-008-7653	I	Si O ₂	Silicon Oxide	quartz low	3.330030	4.235900	1.810760	H	4.8912		5.388			
04-008-7654	I	Si O ₂	Silicon Oxide	quartz low	3.316550	4.216760	1.803590	H	4.8691		5.3703			
04-008-7655	I	Si O ₂	Silicon Oxide	quartz low	3.314940	4.215640	1.802640	H	4.8678		5.3658			
04-008-8228	P	Si O ₂	Silicon Oxide	quartz low	3.342810	4.254350	1.817550	H	4.9125		5.4042			
04-012-0490	I	Si O ₂	Silicon Oxide	Quartz	3.343930	4.255880	1.818150	H	4.9143		5.4058			
04-014-3910	I	Be _{0.94} F _{1.88}	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))}

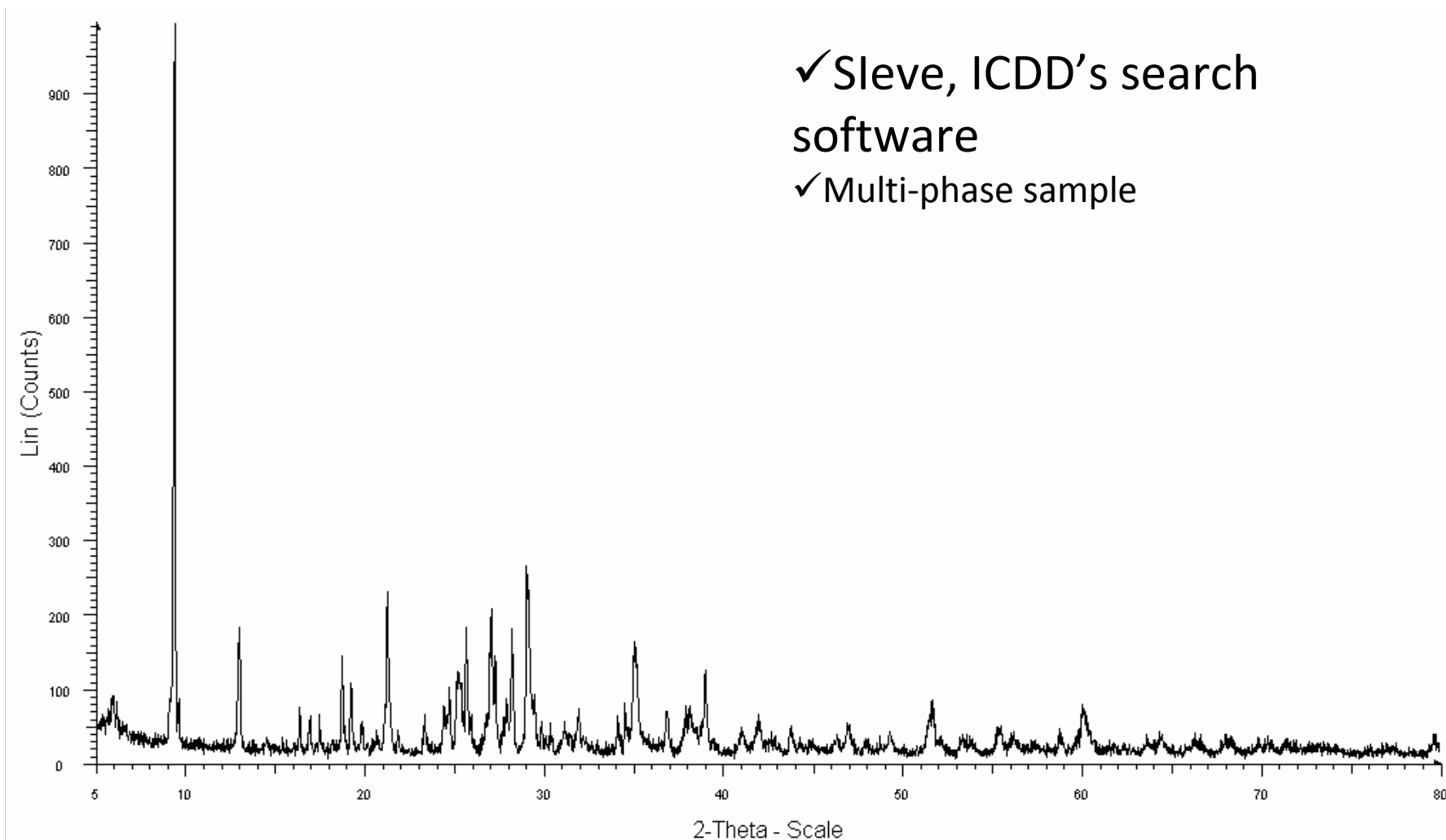
Calculations

Mean: Median: ESD:

[illegible]

4	5.5	2.95	3.03	$\frac{1}{2} \ln A$	$\frac{1}{2}$	$\frac{1}{2} \ln A$	$\frac{1}{2}$
$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.5
1	50	50	40	0.7	0.70	0.70	0.7
				0.8	0.80	0.80	0.8
				0.9	0.90	0.90	0.9
				1.0	1.00	1.00	1.0
				1.1	1.10	1.10	1.1
				1.2	1.20	1.20	1.2
				1.3	1.30	1.30	1.3
				1.4	1.40	1.40	1.4
				1.5	1.50	1.50	1.5
				1.6	1.60	1.60	1.6
				1.7	1.70	1.70	1.7
				1.8	1.80	1.80	1.8
				1.9	1.90	1.90	1.9
				2.0	2.00	2.00	2.0
				2.1	2.10	2.10	2.1
				2.2	2.20	2.20	2.2
				2.3	2.30	2.30	2.3
				2.4	2.40	2.40	2.4
				2.5	2.50	2.50	2.5
				2.6	2.60	2.60	2.6
				2.7	2.70	2.70	2.7
				2.8	2.80	2.80	2.8
				2.9	2.90	2.90	2.9
				3.0	3.00	3.00	3.0
				3.1	3.10	3.10	3.1
				3.2	3.20	3.20	3.2
				3.3	3.30	3.30	3.3
				3.4	3.40	3.40	3.4
				3.5	3.50	3.50	3.5
				3.6	3.60	3.60	3.6
				3.7	3.70	3.70	3.7
				3.8	3.80	3.80	3.8
				3.9	3.90	3.90	3.9
				4.0	4.00	4.00	4.0
				4.1	4.10	4.10	4.1
				4.2	4.20	4.20	4.2
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				4.5	4.50	4.50	4.5
				4.6	4.60	4.60	4.6
				4.7	4.70	4.70	4.7
				4.8	4.80	4.80	4.8
				4.9	4.90	4.90	4.9
				5.0	5.00	5.00	5.0
				5.1	5.10	5.10	5.1
				5.2	5.20	5.20	5.2
				5.3	5.30	5.30	5.3
				5.4	5.40	5.40	5.4
				5.5	5.50	5.50	5.5
				5.6	5.60	5.60	5.6
				5.7	5.70	5.70	5.7
				5.8	5.80	5.80	5.8
				5.9	5.90	5.90	5.9
				6.0	6.00	6.00	6.0
				6.1	6.10	6.10	6.1
				6.2	6.20	6.20	6.2
				6.3	6.30	6.30	6.3
				6.4	6.40	6.40	6.4
				6.5	6.50	6.50	6.5
				6.6	6.60	6.60	6.6
				6.7	6.70	6.70	6.7
				6.8	6.80	6.80	6.8
				6.9	6.90	6.90	6.9
				7.0	7.00	7.00	7.0
				7.1	7.10	7.10	7.1
				7.2	7.20	7.20	7.2
				7.3	7.30	7.30	7.3
				7.4	7.40	7.40	7.4
				7.5	7.50	7.50	7.5
				7.6	7.60	7.60	7.6
				7.7	7.70	7.70	7.7
				7.8	7.80	7.80	7.8
				7.9	7.90	7.90	7.9
				8.0	8.00	8.00	8.0
				8.1	8.10	8.10	8.1
				8.2	8.20	8.20	8.2
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				8.4	8.40	8.40	8.4
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				8.8	8.80	8.80	8.8
				8.9	8.90	8.90	8.9
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				9.1	9.10	9.10	9.1
				9.2	9.20	9.20	9.2
				9.3	9.30	9.30	9.3
				9.4	9.40	9.40	9.4
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				9.8	9.80	9.80	9.8
				9.9	9.90	9.90	9.9
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				10.1	10.10	10.10	10.1
				10.2	10.20	10.20	10.2
				10.3	10.30	10.30	10.3
				10.4	10.40	10.40	10.4
				10.5	10.50	10.50	10.5
				10.6	10.60	10.60	10.6
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				11.0	11.00	11.00	11.0
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				11.2	11.20	11.20	11.2
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				11.5	11.50	11.50	11.5
				11.6	11.60	11.60	11.6
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				11.9	11.90	11.90	11.9
				12.0	12.00	12.00	12.0
				12.1	12.10	12.10	12.1
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				15.1	15.10	15.10	15.1
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				15.5	15.50	15.50	15.5
				15.6	15.60	15.60	15.6
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				15.8	15.80	15.80	15.8
				15.9	15.90	15.90	15.9
				16.0	16.00	16.00	16.0
				16.1	16.10	16.10	16.1
				16.2	16.20	16.20	16.2
				16.3	16.30	16.30	16.3
				16.4	16.40	16.40	16.4
				16.5	16.50	16.50	16.5
				16.6	16.60	16.60	16.6
				16.7	16.70	16.70	16.7
				16.8	16.80	16.80	16.8
				16.9	16.90	16.90	16.9
				17.0	17.00	17.00	17.0
				17.1	17.10	17.10	17.1
				17.2	17.20	17.20	17.2
				17.3	17.30	17.30	17.3
				17.4	17.40	17.40	17.4
				17.5	17.50	17.50	17.5
				17.6	17.60	17.60	17.6
				17.7	17.70	17.70	17.7
				17.8	17.80	17.80	17.8
				17.9	17.90	17.90	17.9
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				18.1	18.10	18.10	18.1
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				18.9	18.90	18.90	18.9
				19.0	19.00	19.00	19.0
				19.1	19.10	19.10	19.1
				19.2	19.20	19.20	19.2
				19.3	19.30	19.30	19.3
				19.4	19.40	19.40	19.4
				19.5	19.50	19.50	19.5
				19.6	19.60	19.60	19.6
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				19.8	19.80	19.80	19.8
				19.9	19.90	19.90	19.9
				20.0	20.00	20.00	20.0
				20.1	20.10	20.10	20.1
				20.2	20.20	20.20	20.2
				20.3	20.30	20.30	20.3
				20.4	20.40	20.40	20.4
				20.5	20.50	20.50	20.5
				20.6	20.60	20.60	20.6
				20.7	20.70	20.70	20.7
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				20.9	20.90	20.90	20.9
				21.0	21.00	21.00	21.0
				21.1	21.10	21.10	21.1
				21.2	21.20	21.20	21.2
				21.3	21.30	21.30	21.3
				21.4	21.40	21.40	21.4
				21.5	21.50	21.50	21.5
				21.6	21.60	21.60	21.6
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				21.8	21.80	21.80	21.8
				21.9	21.90	21.90	21.9
				22.0	22.00	22.00	22.0
				22.1	22.10	22.10	22.1
				22.2	22.20	22.20	22.2
				22.3	22.30		

Example 4



- ✓ Sleve, ICDD's search software

- ✓ Multi-phase sample

d	5.5	2.95	3.03
$\frac{1}{d^2}$	1.00	1.00	1.00
$\frac{1}{d}$	50	50	50
(Cu_2O)			
a	3.57	3.57	3.57
b	3.57	3.57	3.57
c	3.57	3.57	3.57
V	3.57	3.57	3.57
Z	3.57	3.57	3.57
ρ	3.57	3.57	3.57
μ	3.57	3.57	3.57
κ	3.57	3.57	3.57
λ	3.57	3.57	3.57
θ	3.57	3.57	3.57
2θ	3.57	3.57	3.57
$\Delta 2\theta$	3.57	3.57	3.57
Δd	3.57	3.57	3.57
$\Delta \frac{1}{d^2}$	3.57	3.57	3.57
$\Delta \frac{1}{d}$	3.57	3.57	3.57

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)

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

Boolean Yes/No/Maybe

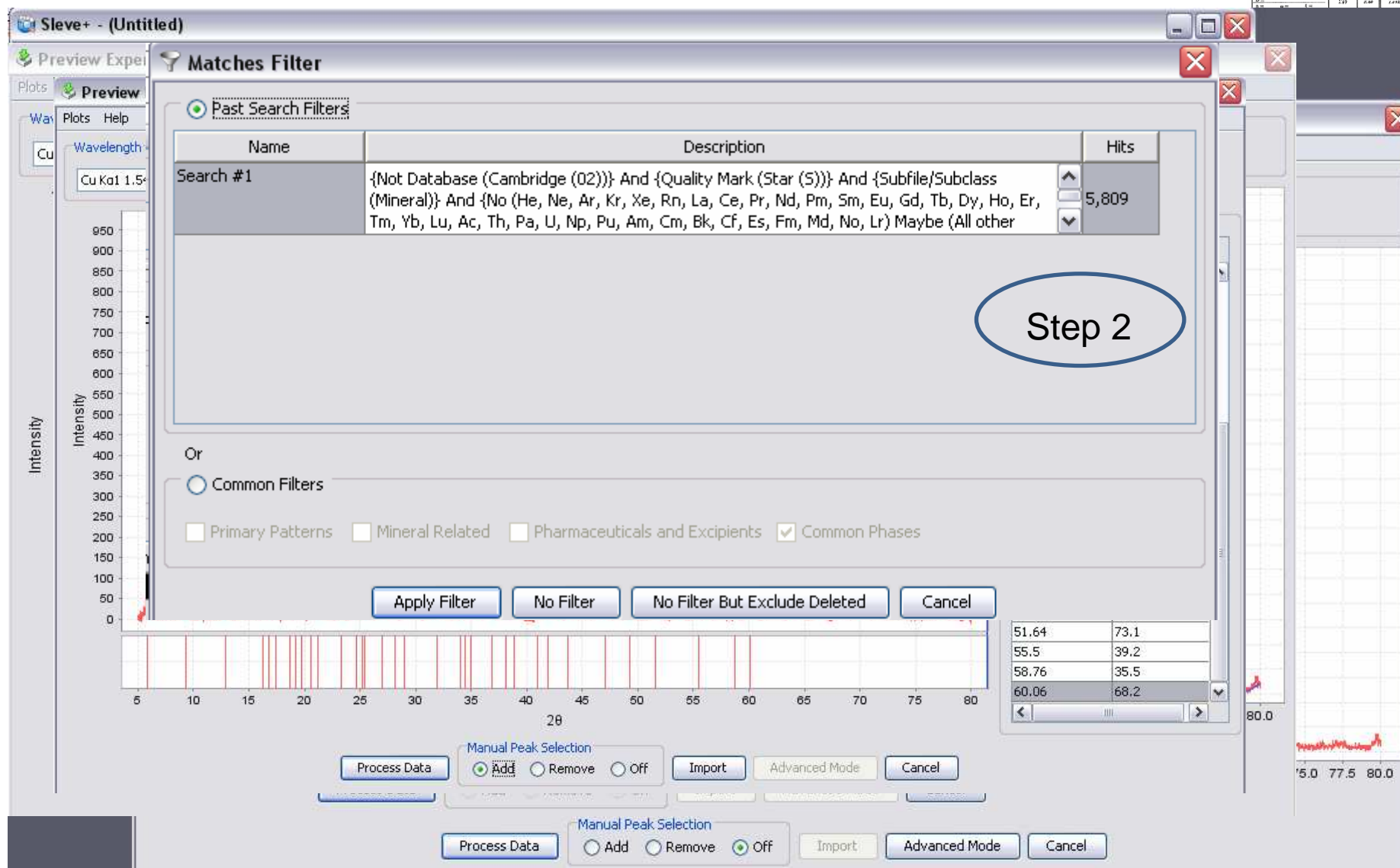
No (He, Ne, Ar, Kr, Xe, Rn, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) Maybe (All other elements)

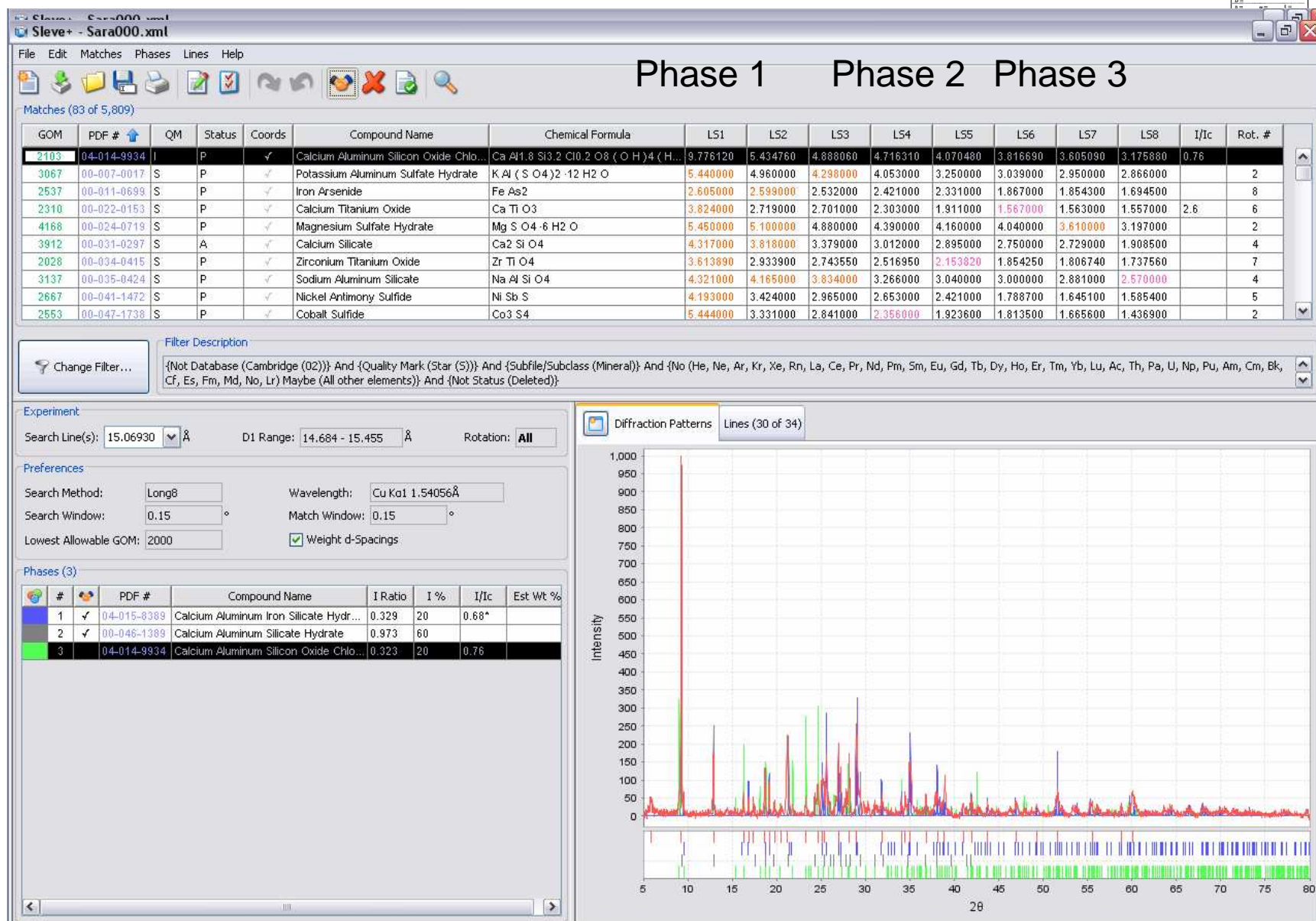
Set Unselected to 'No'

Period	IA	IIA	IIIB	IVB	VB	VIB	VII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA		
1	1 H 1.008															2 He 4.003		
2	3 Li 6.941	4 Be 9.012																
3	11 Na 22.990	12 Mg 24.305																
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 58.933	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]																
LN:	57 La 138.906	58 Ce 140.116	59 Pr 140.908	60 Nd 144.242	61 Pm [146]	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 [268]	102 No [269]	103 Lr [262]			

Search Show Results Undo Page Reset Page Reset All

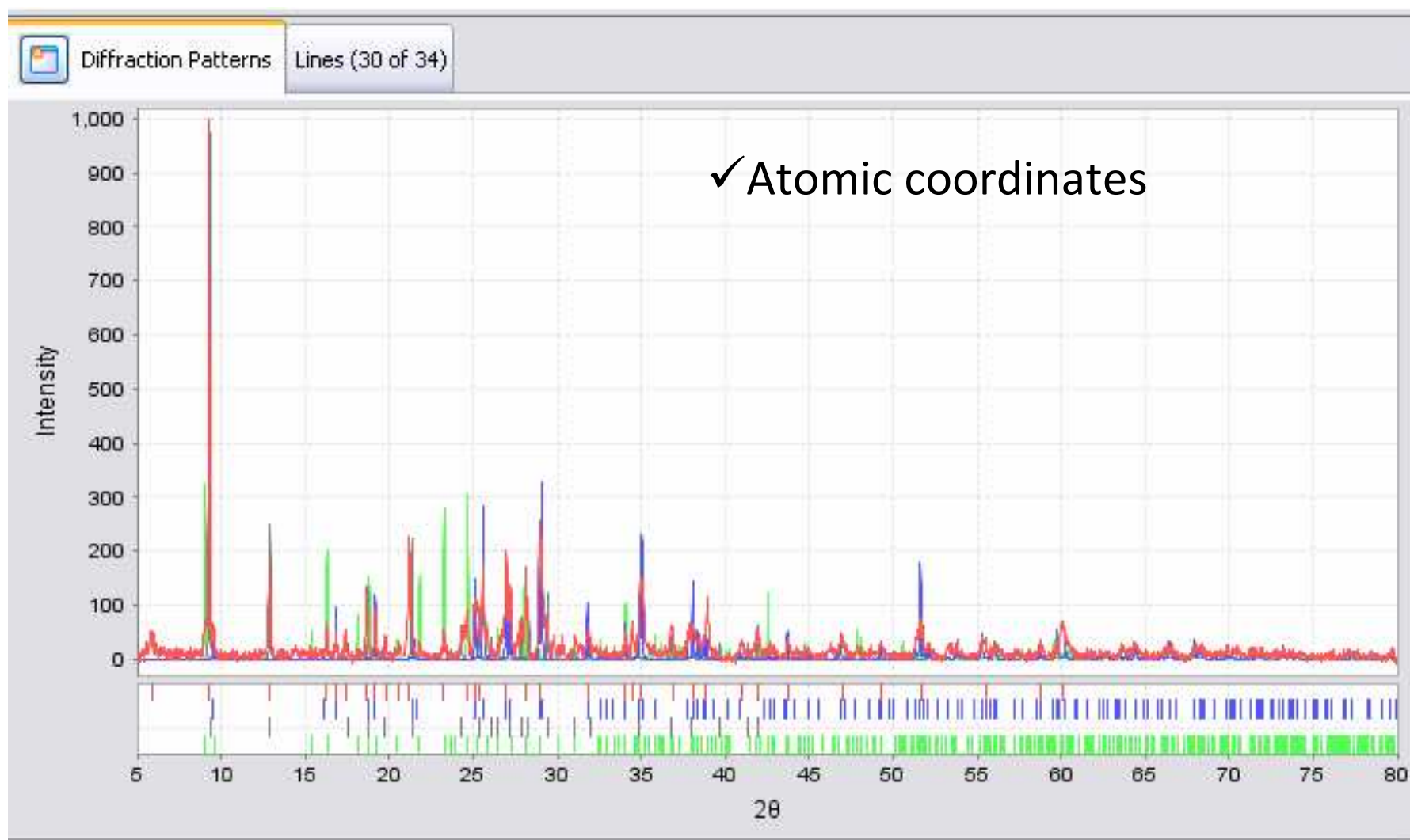
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$\frac{1}{2}$	1.00	1.00	1.00	0.5	0.50	0.50	0.50
1	50	50	40	0.7	0.70	0.70	0.70
				0.8	0.80	0.80	0.80
				0.9	0.90	0.90	0.90
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				1.1	1.10	1.10	1.10
				1.2	1.20	1.20	1.20
				1.3	1.30	1.30	1.30
				1.4	1.40	1.40	1.40
				1.5	1.50	1.50	1.50
				1.6	1.60	1.60	1.60
				1.7	1.70	1.70	1.70
				1.8	1.80	1.80	1.80
				1.9	1.90	1.90	1.90
				2.0	2.00	2.00	2.00
				2.1	2.10	2.10	2.10
				2.2	2.20	2.20	2.20
				2.3	2.30	2.30	2.30
				2.4	2.40	2.40	2.40
				2.5	2.50	2.50	2.50
				2.6	2.60	2.60	2.60
				2.7	2.70	2.70	2.70
				2.8	2.80	2.80	2.80
				2.9	2.90	2.90	2.90
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				3.5	3.50	3.50	3.50
				3.6	3.60	3.60	3.60
				3.7	3.70	3.70	3.70
				3.8	3.80	3.80	3.80
				3.9	3.90	3.90	3.90
				4.0	4.00	4.00	4.00
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				4.8	4.80	4.80	4.80
				4.9	4.90	4.90	4.90
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				5.1	5.10	5.10	5.10
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				5.3	5.30	5.30	5.30
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				5.7	5.70	5.70	5.70
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				15.3	15.30	15.30	15.30
				15.4	15.40	15.40	15.40
				15.5	15.50	15.50	15.50
				15.6	15.60	15.60	15.60
				15.7	15.70	15.70	15.70
				15.8	15.80	15.80	15.80
				15.9	15.90	15.90	15.90
				16.0	16.00	16.00	16.00
				16.1	16.10	16.10	16.10
				16.2	16.20	16.20	16.20
				16.3	16.30	16.30	16.30
				16.4	16.40	16.40	16.40
				16.5	16.50	16.50	16.50
				16.6	16.60	16.60	16.60
				16.7	16.70	16.70	16.70
				16.8	16.80	16.80	16.80
				16.9	16.90	16.90	16.90
				17.0	17.00	17.00	17.00
				17.1	17.10	17.10	17.10
				17.2	17.20	17.20	17.20
				17.3	17.30	17.30	17.30
				17.4	17.40	17.40	17.40
				17.5	17.50	17.50	17.50
				17.6	17.60	17.60	17.60
				17.7	17.70	17.70	17.70
				17.8	17.80	17.80	17.80
				17.9	17.90	17.90	17.90
				18.0	18.00	18.00	18.00
				18.1	18.10	18.10	18.10
				18.2	18.20	18.20	18.20
				18.3	18.30	18.30	18.30
				18.4	18.40	18.40	18.40
				18.5	18.50	18.50	18.50
				18.6	18.60	18.60	18.60
				18.7	18.70	18.70	18.70
				18.8	18.80	18.80	18.80
				18.9	18.90	18.90	18.90
				19.0	19.00	19.00	19.00
				19.1	19.10	19.10	19.10
				19.2	19.20	19.20	19.20
				19.3	19.30	19.30	19.30
				19.4	19.40	19.40	19.40
				19.5	19.50	19.50	19.50
				19.6	19.60	19.60	19.60
				19.7	19.70	19.70	19.70
				19.8	19.80	19.80	19.80
				19.9	19.90	19.90	19.90
				20.0	20.00	20.00	20.00
				20.1	20.10	20.10	20.10
				20.2	20.20	20.20	20.20
				20.3	20.30	20.30	20.30
				20.4	20.40	20.40	20.40
				20.5	20.50	20.50	20.50
				20.6	20.60	20.60	20.60
				20.7	20.70	20.70	20.70
				20.8	20.80	20.80	20.80
				20.9	20.90	20.90	20.90
				21.0	21.00	21.00	21.00
				21.1	21.10	21.10	21.10
				21.2	21.20	21.20	21.20
				21.3	21.30	21.30	21.30
				21.4	21.40	21.40	21.40
				21.5	21.50	21.50	21.50
				21.6	21.60	21.60	21.60
				21.7	21.70	21.70	21.70
				21.8	21.80	21.80	21.80
				21.9	21.90	21.90	21.90</





d	5.5	2.95	3.03	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$
$\frac{1}{\lambda}$	1.00	1.00	0.90	0.2	0.001	0.15	0.001
l	50	50	40	0.3	0.002	0.17	0.002
				0.4	0.003	0.18	0.003
				0.5	0.004	0.19	0.004
				0.6	0.005	0.20	0.005
				0.7	0.006	0.21	0.006
				0.8	0.007	0.22	0.007
				0.9	0.008	0.23	0.008
				1.0	0.009	0.24	0.009
				1.1	0.010	0.25	0.010
				1.2	0.011	0.26	0.011
				1.3	0.012	0.27	0.012
				1.4	0.013	0.28	0.013
				1.5	0.014	0.29	0.014
				1.6	0.015	0.30	0.015
				1.7	0.016	0.31	0.016
				1.8	0.017	0.32	0.017
				1.9	0.018	0.33	0.018
				2.0	0.019	0.34	0.019
				2.1	0.020	0.35	0.020
				2.2	0.021	0.36	0.021
				2.3	0.022	0.37	0.022
				2.4	0.023	0.38	0.023
				2.5	0.024	0.39	0.024
				2.6	0.025	0.40	0.025
				2.7	0.026	0.41	0.026
				2.8	0.027	0.42	0.027
				2.9	0.028	0.43	0.028
				3.0	0.029	0.44	0.029
				3.1	0.030	0.45	0.030
				3.2	0.031	0.46	0.031
				3.3	0.032	0.47	0.032
				3.4	0.033	0.48	0.033
				3.5	0.034	0.49	0.034
				3.6	0.035	0.50	0.035
				3.7	0.036	0.51	0.036
				3.8	0.037	0.52	0.037
				3.9	0.038	0.53	0.038
				4.0	0.039	0.54	0.039
				4.1	0.040	0.55	0.040
				4.2	0.041	0.56	0.041
				4.3	0.042	0.57	0.042
				4.4	0.043	0.58	0.043
				4.5	0.044	0.59	0.044
				4.6	0.045	0.60	0.045
				4.7	0.046	0.61	0.046
				4.8	0.047	0.62	0.047
				4.9	0.048	0.63	0.048
				5.0	0.049	0.64	0.049
				5.1	0.050	0.65	0.050
				5.2	0.051	0.66	0.051
				5.3	0.052	0.67	0.052
				5.4	0.053	0.68	0.053
				5.5	0.054	0.69	0.054
				5.6	0.055	0.70	0.055
				5.7	0.056	0.71	0.056
				5.8	0.057	0.72	0.057
				5.9	0.058	0.73	0.

Example 5



h	k	l	2θ	d	I	h	k	l	2θ	d	I
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100
1	0	0	1.00	1.00	100	1	0	0	1.00	1.00	100

Ca₂ Fe_{0.26} Al_{1.74} Si₃ O₁₀ (OH)

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Save

04-015-8389

Mar 28, 2013 10:17 AM (jgil)

Status: Alternate QM: Star(S) Pressure/Temperature: Ambient

Chemical Formula: Ca₂ Fe_{0.26} Al_{1.74} Si₃ O₁₀ (OH)₂ Empirical Formula: Al_{1.74} Ca₂ Fe_{0.26} H₂ O₁₂ Si₃

Weight %: Al11.18 Ca19.09 Fe3.48 H0.43 O45.72 Si20.07 Atomic %: Al8.29 Ca29.52 Fe1.24 H0.32 O57.14 Si14.29

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: Crystal Optical Structure Miscellaneous

Compound Name: Calcium A

Mineral Name: prehnite

Common Name:

CIF (2θ, I pairs) (*.cif)

CIF (I, 10 per record) (*.cif)

ICDD Delimited text (*.csv)

ICDD Formatted text (*.prn)

ICDD XML (*.xml)

a	b	c	β	γ	V	Z	ρ	ρ_c	ρ_x
Å	Å	Å	°	°	Å ³		g/cm ³	g/cm ³	g/cm ³
1.00	1.00	1.00	90	90	1.000	1	0.000	0.000	0.000
1.50	1.50	1.50	90	90	3.375	1	0.000	0.000	0.000
2.00	2.00	2.00	90	90	8.000	1	0.000	0.000	0.000
2.50	2.50	2.50	90	90	15.625	1	0.000	0.000	0.000
3.00	3.00	3.00	90	90	27.000	1	0.000	0.000	0.000
3.50	3.50	3.50	90	90	42.875	1	0.000	0.000	0.000
4.00	4.00	4.00	90	90	64.000	1	0.000	0.000	0.000
4.50	4.50	4.50	90	90	91.125	1	0.000	0.000	0.000
5.00	5.00	5.00	90	90	125.000	1	0.000	0.000	0.000
5.50	5.50	5.50	90	90	166.375	1	0.000	0.000	0.000
6.00	6.00	6.00	90	90	216.000	1	0.000	0.000	0.000
6.50	6.50	6.50	90	90	274.625	1	0.000	0.000	0.000
7.00	7.00	7.00	90	90	343.000	1	0.000	0.000	0.000
7.50	7.50	7.50	90	90	421.875	1	0.000	0.000	0.000
8.00	8.00	8.00	90	90	512.000	1	0.000	0.000	0.000
8.50	8.50	8.50	90	90	614.625	1	0.000	0.000	0.000
9.00	9.00	9.00	90	90	729.000	1	0.000	0.000	0.000
9.50	9.50	9.50	90	90	857.375	1	0.000	0.000	0.000
10.00	10.00	10.00	90	90	1000.000	1	0.000	0.000	0.000

Inorganic Crystal Structural Database

Information center FIZ Karlsruhe

✓ Inorganic Structures







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



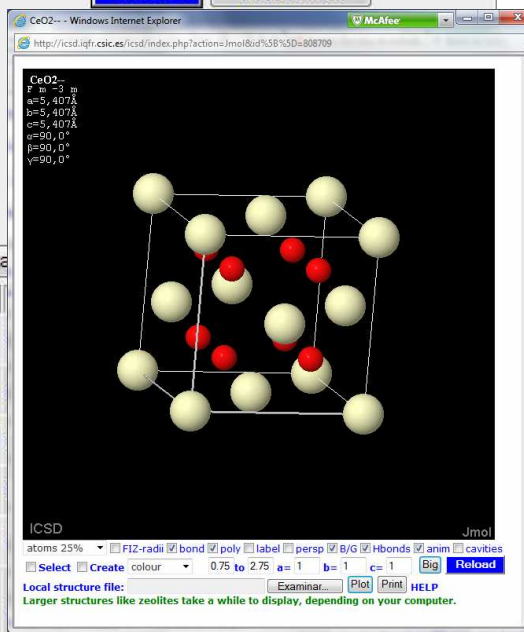
- Structural data
- Atomic coordinates
- Bibliographic data
- Synthesis conditions

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

Windows Internet Explorer    

Det

	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 Ce _{1-x} Gd _x O _{2-x/2} using the pair distribution function analysis
ier, J.;	Structural characterization of the CeO ₂ / Gd ₂ O ₃ mixed system by synchrotron X-ray diffraction
leukoo;	Dopant induced variations in microstructure and optical properties of CeO ₂ nanoparticles
ig; a.Dic	Facile hydrothermal synthesis of CeO ₂ nanosheets with high reactive



2 nanospheres self-

- x Prx O2-delta as an

-x Prx O2-delta as an

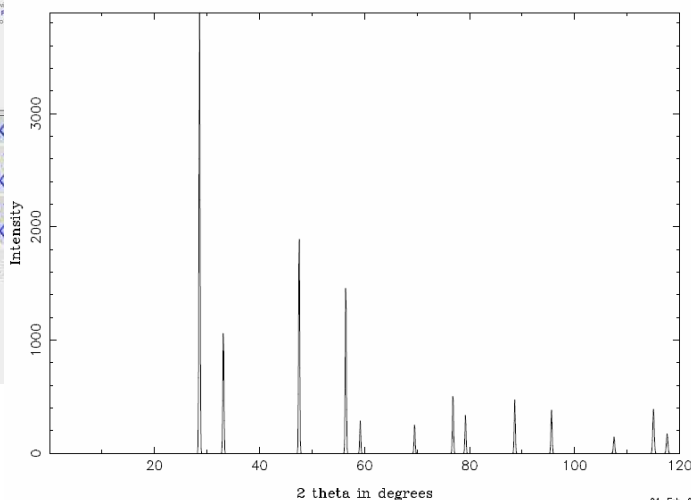
ologist database

le after the first query is

by Peter Hewat email: hp@fz-karlsruhe.de

References

tion Database



21-Feb-2013 14:12

[illegible]

a	5.5	2.95	3.03	$a^* \sin \alpha$	1	$a^* \sin \beta$	1
b	1.00	1.00	0.80	$b^* \sin \alpha$	1	$b^* \sin \beta$	1
c	50	50	40	$c^* \sin \alpha$	1	$c^* \sin \beta$	1
$(C_{2v}(C_2))$				V	1	V	1
				Z	1	Z	1
				R	1	R	1
				wR	1	wR	1
				S	1	S	1
				χ^2	1	χ^2	1
				σ	1	σ	1
				μ	1	μ	1
				ρ	1	ρ	1
				ρ_{max}	1	ρ_{max}	1
				ρ_{min}	1	ρ_{min}	1
				ρ_{avg}	1	ρ_{avg}	1
				ρ_{std}	1	ρ_{std}	1
				ρ_{total}	1	ρ_{total}	1
				ρ_{total}^2	1	ρ_{total}^2	1
				ρ_{total}^3	1	ρ_{total}^3	1
				ρ_{total}^4	1	ρ_{total}^4	1
				ρ_{total}^5	1	ρ_{total}^5	1
				ρ_{total}^6	1	ρ_{total}^6	1
				ρ_{total}^7	1	ρ_{total}^7	1
				ρ_{total}^8	1	ρ_{total}^8	1
				ρ_{total}^9	1	ρ_{total}^9	1
				ρ_{total}^{10}	1	ρ_{total}^{10}	1

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

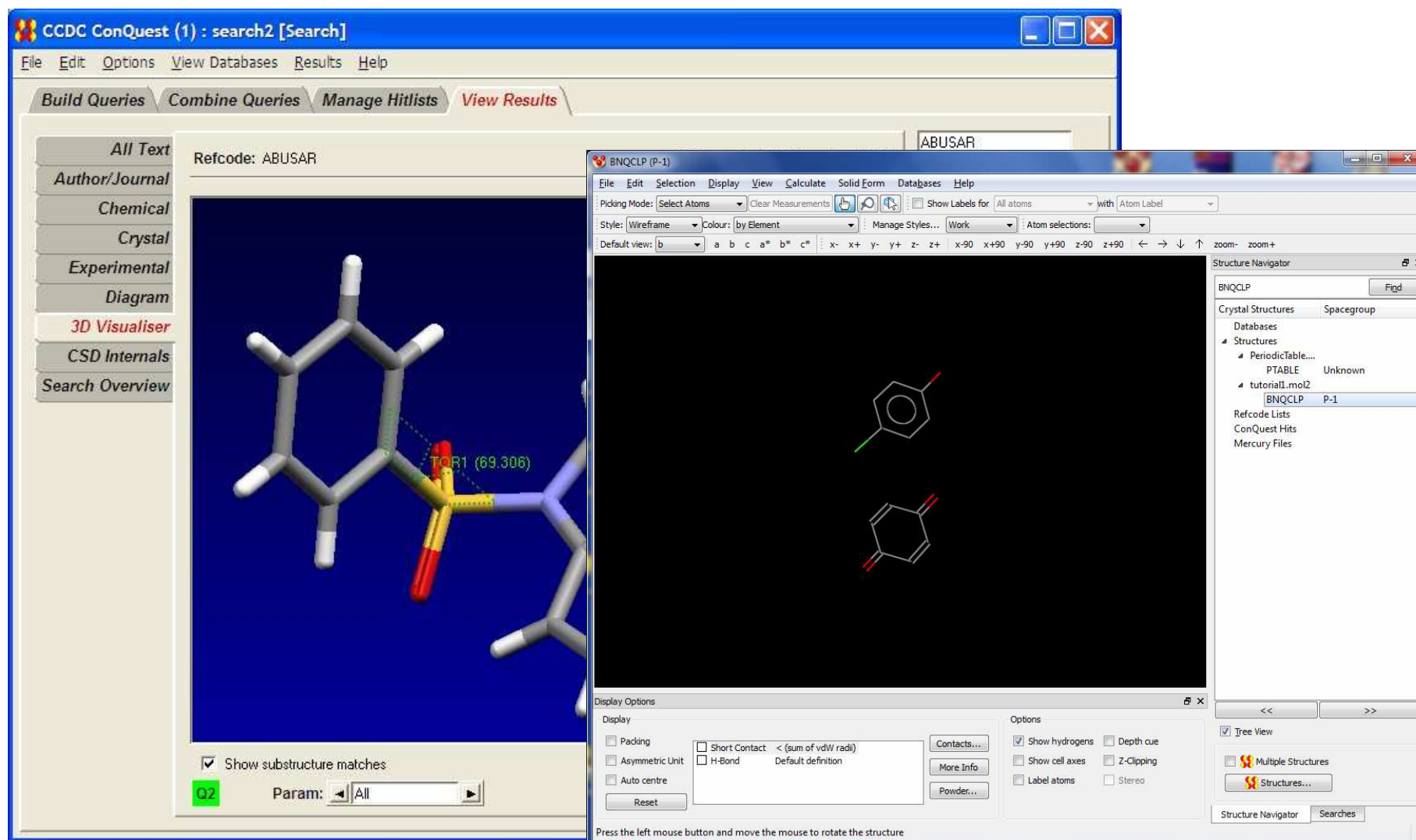
- ❖ Software version
 - ✓ software for search and information retrieval (ConQuest)
 - ✓ structure visualisation (Mercury)
 - ✓ numerical analysis (Vista)
 - ✓ database creation (PreQuest)

❖ WebCSD

(Access requires personal registration)

d	5.5	295	3.03	$d \sin \lambda$	$\frac{1}{\lambda}$	$d \sin \lambda$	$\frac{1}{\lambda}$
$\frac{1}{\lambda}$	1.00	1.00	0.80	0.8	1.25	1.12	0.89
				0.7	1.43	1.04	0.96
				0.6	1.67	0.96	1.04
t	50	50	40	0.5	2.00	0.88	1.13
$(e_{\lambda}(SO_2)_t)$				0.45	2.22	0.86	1.15
				0.4	2.50	0.84	1.19
				0.35	2.86	0.82	1.23
				0.3	3.33	0.80	1.28
				0.25	4.00	0.76	1.37
				0.2	5.00	0.72	1.48
				0.15	6.67	0.67	1.64
				0.1	10.00	0.60	1.67
				0.05	20.00	0.50	2.00
				0.02	50.00	0.40	2.50
				0.01	100.00	0.30	3.33
				0.005	200.00	0.20	5.00
				0.002	500.00	0.15	6.67
				0.001	1000.00	0.10	10.00
				0.0005	2000.00	0.05	20.00
				0.0002	5000.00	0.02	50.00
				0.0001	10000.00	0.01	100.00
				0.00005	20000.00	0.005	200.00
				0.00002	50000.00	0.002	500.00
				0.00001	100000.00	0.001	1000.00
				0.000005	200000.00	0.0005	2000.00
				0.000002	500000.00	0.0002	5000.00
				0.000001	1000000.00	0.0001	10000.00
				0.0000005	2000000.00	0.00005	20000.00
				0.0000002	5000000.00	0.00002	50000.00
				0.0000001	10000000.00	0.00001	100000.00
				0.00000005	20000000.00	0.000005	200000.00
				0.00000002	50000000.00	0.000002	500000.00
				0.00000001	100000000.00	0.000001	1000000.00
				0.000000005	200000000.00	0.0000005	2000000.00
				0.000000002	500000000.00	0.0000002	5000000.00
				0.000000001	1000000000.00	0.0000001	10000000.00
				0.0000000005	2000000000.00	0.00000005	20000000.00
				0.0000000002	5000000000.00	0.00000002	50000000.00
				0.0000000001	10000000000.00	0.00000001	100000000.00
				0.00000000005	20000000000.00	0.000000005	200000000.00
				0.00000000002	50000000000.00	0.000000002	500000000.00
				0.00000000001	100000000000.00	0.000000001	1000000000.00
				0.000000000005	200000000000.00	0.0000000005	2000000000.00
				0.000000000002	500000000000.00	0.0000000002	5000000000.00
				0.000000000001	1000000000000.00	0.0000000001	10000000000.00
				0.0000000000005	2000000000000.00	0.00000000005	20000000000.00
				0.0000000000002	5000000000000.00	0.00000000002	50000000000.00
				0.0000000000001	10000000000000.00	0.00000000001	100000000000.00
				0.00000000000005	20000000000000.00	0.000000000005	200000000000.00
				0.00000000000002	50000000000000.00	0.000000000002	500000000000.00
				0.00000000000001	100000000000000.00	0.000000000001	1000000000000.00
				0.000000000000005	200000000000000.00	0.0000000000005	2000000

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



d	5.5	2.95	3.03	$d \pm \Delta$	$\frac{1}{d}$	$d \pm \Delta$	$\frac{1}{d}$
$\frac{1}{d}$	1.00	1.00	0.90	5.5	0.182	5.5	0.182
$\frac{1}{d}$	50	50	40	4.7	0.213	4.7	0.213
				2.3	0.435	2.3	0.435
				1.95	0.513	1.95	0.513
				1.7	0.588	1.7	0.588
				1.57	0.637	1.57	0.637
				1.46	0.685	1.46	0.685
				1.37	0.729	1.37	0.729
				1.3	0.769	1.3	0.769
				1.23	0.813	1.23	0.813
				1.17	0.854	1.17	0.854
				1.12	0.893	1.12	0.893
				1.07	0.935	1.07	0.935
				1.03	0.971	1.03	0.971
				1.00	1.000	1.00	1.000
				0.97	1.031	0.97	1.031
				0.94	1.064	0.94	1.064
				0.91	1.099	0.91	1.099
				0.88	1.136	0.88	1.136
				0.86	1.165	0.86	1.165
				0.84	1.196	0.84	1.196
				0.82	1.229	0.82	1.229
				0.80	1.264	0.80	1.264
				0.78	1.299	0.78	1.299
				0.76	1.336	0.76	1.336
				0.74	1.375	0.74	1.375
				0.72	1.417	0.72	1.417
				0.70	1.461	0.70	1.461
				0.68	1.507	0.68	1.507
				0.66	1.556	0.66	1.556
				0.64	1.607	0.64	1.607
				0.62	1.660	0.62	1.660
				0.60	1.717	0.60	1.717
				0.58	1.777	0.58	1.777
				0.56	1.840	0.56	1.840
				0.54	1.907	0.54	1.907
				0.52	1.979	0.52	1.979
				0.50	2.057	0.50	2.057
				0.48	2.140	0.48	2.140
				0.46	2.228	0.46	2.228
				0.44	2.321	0.44	2.321
				0.42	2.420	0.42	2.420
				0.40	2.525	0.40	2.525
				0.38	2.637	0.38	2.637
				0.36	2.756	0.36	2.756
				0.34	2.883	0.34	2.883

Crystal Data File

NIST- National Institute of Standards and Technology

✓ Unit cell of crystalline materials



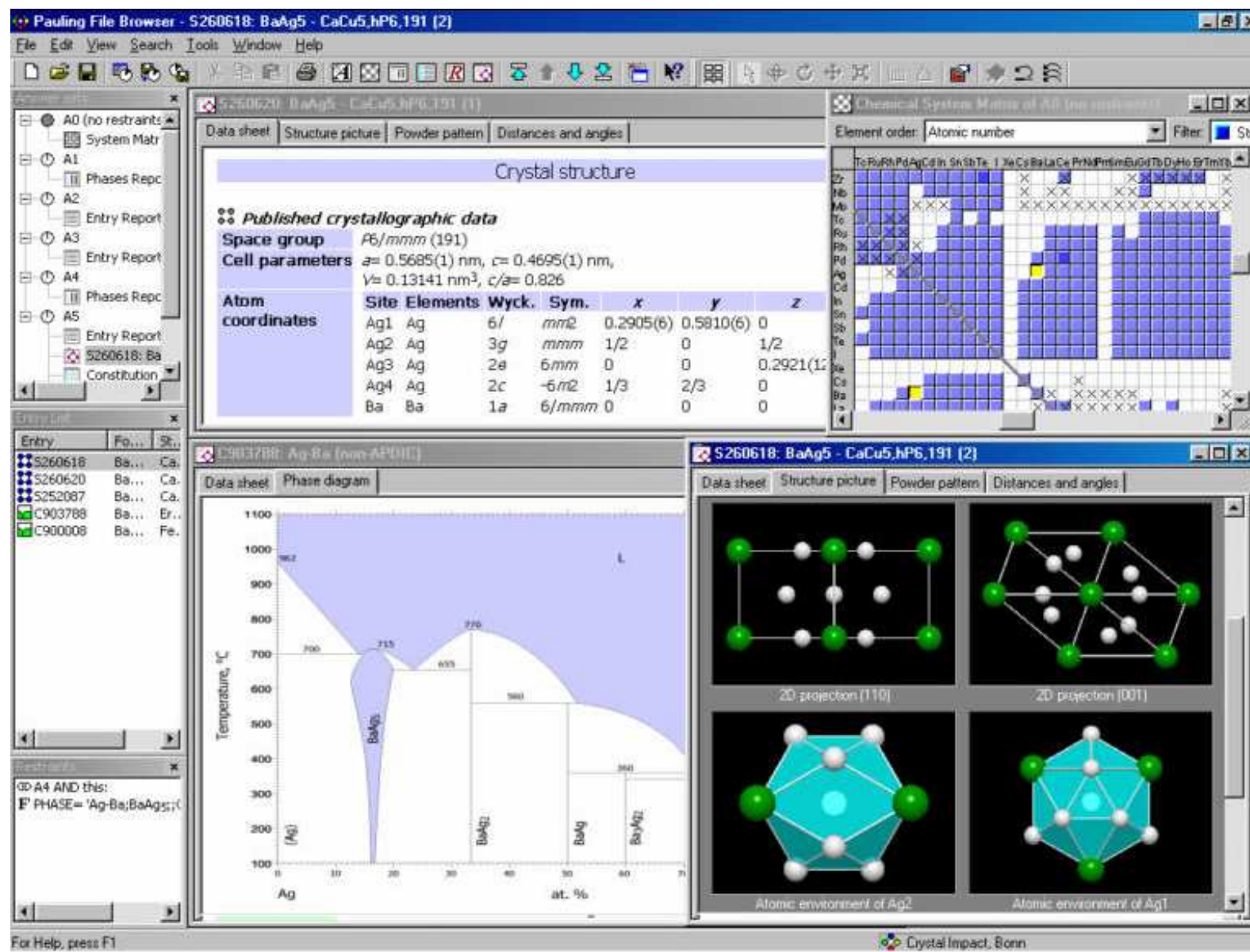
237000 entries



- 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)

[illegible]

d	5.5	2.95	3.03	$d \pm \Delta$	$\frac{1}{d}$	$d \pm \Delta$	$\frac{1}{d}$
$\frac{1}{d}$	1.00	1.00	0.90	2.9	2.62	1.72	2.62
				4.7	2.12	1.72	2.12
				8.3	1.20	1.25	1.20
				14.6	0.68	0.68	0.68
				26.7	0.37	0.37	0.37
				47.0	0.21	0.21	0.21
				83.0	0.12	0.12	0.12
				146.0	0.068	0.068	0.068
				267.0	0.037	0.037	0.037
				470.0	0.021	0.021	0.021
				830.0	0.012	0.012	0.012
				1460.0	0.0068	0.0068	0.0068
				2670.0	0.0037	0.0037	0.0037
				4700.0	0.0021	0.0021	0.0021
				8300.0	0.0012	0.0012	0.0012
				14600.0	0.00068	0.00068	0.00068
				26700.0	0.00037	0.00037	0.00037
				47000.0	0.00021	0.00021	0.00021
				83000.0	0.00012	0.00012	0.00012
				146000.0	0.000068	0.000068	0.000068
				267000.0	0.000037	0.000037	0.000037
				470000.0	0.000021	0.000021	0.000021
				830000.0	0.000012	0.000012	0.000012
				1460000.0	0.0000068	0.0000068	0.0000068
				2670000.0	0.0000037	0.0000037	0.0000037
				4700000.0	0.0000021	0.0000021	0.0000021
				8300000.0	0.0000012	0.0000012	0.0000012
				14600000.0	0.00000068	0.00000068	0.00000068
				26700000.0	0.00000037	0.00000037	0.00000037
				47000000.0	0.00000021	0.00000021	0.00000021
				83000000.0	0.00000012	0.00000012	0.00000012
				146000000.0	0.000000068	0.000000068	0.000000068
				267000000.0	0.000000037	0.000000037	0.000000037
				470000000.0	0.000000021	0.000000021	0.000000021
				830000000.0	0.000000012	0.000000012	0.000000012
				1460000000.0	0.0000000068	0.0000000068	0.0000000068
				2670000000.0	0.0000000037	0.0000000037	0.0000000037
				4700000000.0	0.0000000021	0.0000000021	0.0000000021
				8300000000.0	0.0000000012	0.0000000012	0.0000000012
				14600000000.0	0.00000000068	0.00000000068	0.00000000068
				26700000000.0	0.00000000037	0.00000000037	0.00000000037
				47000000000.0	0.00000000021	0.00000000021	0.00000000021
				83000000000.0	0.00000000012	0.00000000012	0.00000000012
				146000000000.0	0.000000000068	0.000000000068	0.000000000068
				267000000000.0	0.000000000037	0.000000000037	0.000000000037
				470000000000.0	0.000000000021	0.000000000021	0.000000000021
				830000000000.0	0.000000000012	0.000000000012	0.000000000012
				1460000000000.0	0.0000000000068	0.0000000000068	0.0000000000068
				2670000000000.0	0.0000000000037	0.0000000000037	0.0000000000037
				4700000000000.0	0.0000000000021	0.0000000000021	0.0000000000021
				8300000000000.0	0.0000000000012	0.0000000000012	0.0000000000012
				14600000000000.0	0.00000000000068	0.00000000000068	0.00000000000068
				26700000000000.0	0.00000000000037	0.00000000000037	0.00000000000037
				47000000000000.0	0.00000000000021	0.00000000000021	0.00000000000021
				83000000000000.0	0.00000000000012	0.00000000000012	0.00000000000012
				146000000000000.0	0.000000000000068	0.000000000000068	0.000000000000068
				267000000000000.0	0.000000000000037	0.000000000000037	0.000000000000037
				470000000000000.0	0.000000000000021	0.000000000000021	0.000000000000021
				830000000000000.0	0.000000000000012	0.000000000000012	0.000000000000012
				1460000000000000.0	0.0000000000000068	0.0000000000000068	0.0000000000000068
				2670000000000000.0	0.0000000000000037	0.0000000000000037	0.0000000000000037
				4700000000000000.0	0.0000000000000021	0.0000000000000021	0.0000000000000021
				8300000000000000.0	0.0000000000000012	0.0000000000000012	0.0000000000000012
				14600000000000000.0	0.00000000000000068	0.00000000000000068	0.00000000000000068
				26700000000000000.0	0.00000000000000037	0.00000000000000037	0.00000000000000037
				47000000000000000.0	0.00000000000000021	0.00000000000000021	0.00000000000000021
				83000000000000000.0	0.00000000000000012	0.00000000000000012	0.00000000000000012
				146000000000000000.0	0.000000000000000068	0.000000000000000068	0.000000000000000068
				267000000000000000.0	0.000000000000000037	0.000000000000000037	0.000000000000000037
				470000000000000000.0	0.000000000000000021	0.000000000000000021	0.000000000000000021
				830000000000000000.0	0.000000000000000012	0.000000000000000012	0.000000000000000012
				1460000000000000000.0	0.0000000000000000068	0.0000000000000000068	0.0000000000000000068
				2670000000000000000.0	0.0000000000000000037	0.0000000000000000037	0.0000000000000000037
				4700000000000000000.0	0.0000000000000000021	0.0000000000000000021	0.0000000000000000021
				8300000000000000000.0	0.0000000000000000012	0.0000000000000000012	0.0000000000000000012
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				26700000000000000000.0	0.00000000000000000037	0.00000000000000000037	0.00000000000000000037
				47000000000000000000.0	0.00000000000000000021	0.00000000000000000021	0.00000000000000000021
				83000000000000000000.0	0.00000000000000000012	0.00000000000000000012	0.00000000000000000012
				146000000000000000000.0	0.000000000000000000068	0.000000000000000000068	0.000000000000000000068
				267000000000000000000.0	0.000000000000000000037	0.000000000000000000037	0.000000000000000000037
				470000000000000000000.0	0.000000000000000000021	0.000000000000000000021	0.000000000000000000021
				830000000000000000000.0	0.000000000000000000012	0.000000000000000000012	0.000000000000000000012
				1460000000000000000000.0	0.0000000000000000000068	0.0000000000000000000068	0.0000000000000000000068
				2670000000000000000000.0	0.0000000000000000000037	0.0000000000000000000037	0.0000000000000000000037
				4700000000000000000000.0	0.0000000000000000000021	0.0000000000000000000021	0.0000000000000000000021
				8300000000000000000000.0	0.0000000000000000000012	0.0000000000000000000012	0.0000000000000000000012
				14600000000000000000000.0	0.00000000000000000000068	0.00000000000000000000068	0.00000000000000000000068
				26700000000000000000000.0	0.00000000000000000000037	0.00000000000000000000037	0.00000000000000000000037
				47000000000000000000000.0	0.00000000000000000000021	0.00000000000000000000021	0.00000000000000000000021
				83000000000000000000000.0	0.00000000000000000000012	0.00000000000000000000012	0.00000000000000000000012
				146000000000000000000000.0	0.000000000000000000000068	0.000000000000000000000068	0.000000000000000000000068
				267000000000000000000000.0	0.000000000000000000000037	0.000000000000000000000037	0.000000000000000000000037
				470000000000000000000000.0	0.000000000000000000000021	0.000000000000000000000021	0.000000000000000000000021
				830000000000000000000000.0	0.000000000000000000000012	0.000000000000000000000012	0.000000000000000000000012
				1460000000000000000000000.0	0.0000000000000000000000068	0.0000000000000000000000068	0.0000000000000000000000068
				2670000000000000000000000.0	0.0000000000000000000000037	0.0000000000000000000000037	0.0000000000000000000000037
				4700000000000000000000000.0	0.0000000000000000000000021	0.0000000000000000000000021	0.0000000000000000000000021
				8300000000000000000000000.0	0.0000000000000000000000012	0.0000000000000000000000012	0.0000000000000000000000012
				14600000000000000000000000.0	0.00000000000000000000000068	0.00000000000000000000000068	0.00000000000000000000000068
				26700000000000000000000000.0	0.00000000000000000000000037	0.00000000000000000000000037	0.00000000000000000000000037
				47000000000000000000000000.0	0.00000000000000000000000021	0.00000000000000000000000021	0.00000000000000000000000021
				83000000000000000000000000.0	0.00000000000000000000000012	0.00000000000000000000000012	0.00000000000000000000000012
				146000000000000000000000000.0	0.000000000000000000000000068	0.000000000000000000000000068	0.000000000000000000000000068
				267000000000000000000000000.0	0.000000000000000000000000037	0.000000000000000000000000037	0.000000000000000000000000037
				470000000000000000000000000.0	0.000000000000000000000000021	0.000000000000000000000000021	0.000000000000000000000000021
				8300000000000000000000000			

CRYSTMET

Toth Information Systems

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

109,877 entries

- Crystallographic data
- Atomic coordinates
- Calculated powder diffraction patterns



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

[illegible]

CRYSTMET(R) – The Metals Database

File Edit View Help

Search Results

Periodic Table Bibliographic Unit Cell Powder Patterns Formula ID Codes

1A 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

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Hide

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

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

Space Group Name: P 21 21 2



a	5.5	2.95	3.03	d in A	1	d in A	1
1/2	1.00	1.00	1.00	1/2	1.00	1.00	1.00
1	50	50	40	1	50	50	40
(C ₂ SO ₂)				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
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				1	50	50	40
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				1	50	50	40
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				1/2	1.00	1.00	1.00
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				1/2	1.00	1.00	1.00
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				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
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				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
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				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
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				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
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				1	50	50	40
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				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
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				1/2	1.00	1.00	1.00
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				1	50	50	40
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				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00
				1	50	50	40
				1/2	1.00	1.00	1.00



d	$h^2 + k^2 + l^2$	a^2	b^2	c^2	V	d_{calc}	d_{obs}
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.50	4.00	4.00	4.00	4.00	4.00	0.50	0.50
0.33	9.00	9.00	9.00	9.00	9.00	0.33	0.33
0.25	16.00	16.00	16.00	16.00	16.00	0.25	0.25
0.20	25.00	25.00	25.00	25.00	25.00	0.20	0.20
0.16	36.00	36.00	36.00	36.00	36.00	0.16	0.16
0.14	49.00	49.00	49.00	49.00	49.00	0.14	0.14
0.12	64.00	64.00	64.00	64.00	64.00	0.12	0.12
0.11	81.00	81.00	81.00	81.00	81.00	0.11	0.11
0.10	100.00	100.00	100.00	100.00	100.00	0.10	0.10

X-Ray Diffraction Table

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Minerals Arranged by X-Ray Powder Diffraction

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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/I₀), 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 1.54056 - CuKα1	Change X-Ray λ <input type="text"/>	D ₁ Å <input type="text"/>	D ₂ Å <input type="text"/>	D ₃ Å <input type="text"/>	Tolerance % <input type="text"/>	Elements <input type="text"/>	Enviar consulta
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[\[1\]](#) [\[2\]](#) [\[3\]](#) [\[4\]](#) [\[5\]](#) [\[6\]](#) [\[7\]](#) [\[8\]](#) [\[9\]](#) [\[10\]](#) [\[11\]](#) [\[12\]](#) [\[13\]](#) [\[14\]](#) [\[15\]](#) [\[16\]](#) [\[17\]](#) [\[18\]](#) [\[19\]](#) [\[20\]](#) [\[21\]](#) [\[22\]](#) [\[23\]](#) [\[24\]](#) [\[25\]](#) [\[26\]](#) [\[27\]](#) [\[28\]](#) [\[29\]](#) [\[30\]](#) [\[31\]](#) [\[32\]](#)
[\[33\]](#) [\[34\]](#) [\[35\]](#) [\[36\]](#) [\[37\]](#) [\[38\]](#) [\[39\]](#) [\[40\]](#) [\[41\]](#) [\[42\]](#) [\[43\]](#) [\[44\]](#) [\[45\]](#) [\[46\]](#) [\[47\]](#) [\[48\]](#) [\[49\]](#) [\[50\]](#) [\[51\]](#) [\[52\]](#) [\[53\]](#) [\[54\]](#) [\[55\]](#) [\[56\]](#) [\[57\]](#) [\[58\]](#) [\[59\]](#) [\[60\]](#) [\[61\]](#) [\[62\]](#)
[\[63\]](#) [\[64\]](#) [\[65\]](#)



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

d	5.5	2.95	3.03	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$	$\frac{1}{\lambda}$ in Å	$\frac{1}{\lambda}$
$\frac{1}{\lambda}$	1.00	1.00	0.90	0.2	0.001	0.15	0.001
l	50	50	40	0.3	0.001	0.17	0.001
				0.4	0.001	0.18	0.001
				0.5	0.001	0.19	0.001
				0.6	0.001	0.20	0.001
				0.7	0.001	0.21	0.001
				0.8	0.001	0.22	0.001
				0.9	0.001	0.23	0.001
				1.0	0.001	0.24	0.001
				1.1	0.001	0.25	0.001
				1.2	0.001	0.26	0.001
				1.3	0.001	0.27	0.001
				1.4	0.001	0.28	0.001
				1.5	0.001	0.29	0.001
				1.6	0.001	0.30	0.001
				1.7	0.001	0.31	0.001
				1.8	0.001	0.32	0.001
				1.9	0.001	0.33	0.001
				2.0	0.001	0.34	0.001
				2.1	0.001	0.35	0.001
				2.2	0.001	0.36	0.001
				2.3	0.001	0.37	0.001
				2.4	0.001	0.38	0.001
				2.5	0.001	0.39	0.001
				2.6	0.001	0.40	0.001
				2.7	0.001	0.41	0.001
				2.8	0.001	0.42	0.001
				2.9	0.001	0.43	0.001
				3.0	0.001	0.44	0.001
				3.1	0.001	0.45	0.001
				3.2	0.001	0.46	0.001
				3.3	0.001	0.47	0.001
				3.4	0.001	0.48	0.001
				3.5	0.001	0.49	0.001
				3.6	0.001	0.50	0.001
				3.7	0.001	0.51	0.001
				3.8	0.001	0.52	0.001
				3.9	0.001	0.53	0.001
				4.0	0.001	0.54	0.001
				4.1	0.001	0.55	0.001
				4.2	0.001	0.56	0.001
				4.3	0.001	0.57	0.001
				4.4	0.001	0.58	0.001
				4.5	0.001	0.59	0.001
				4.6	0.001	0.60	0.001
				4.7	0.001	0.61	0.001
				4.8	0.001	0.62	0.001
				4.9	0.001	0.63	0.001
				5.0	0.001	0.64	0.001
				5.1	0.001	0.65	0.001
				5.2	0.001	0.66	0.001
				5.3	0.001	0.67	0.001
				5.4	0.001	0.68	0.001
				5.5	0.001	0.69	0.001
				5.6	0.001	0.70	0.001
				5.7	0.001	0.71	0.001
				5.8	0.001	0.72	0.001
				5.9	0.001	0.73	0.

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

[illegible]

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 = 18.524Å		b = 5.0032Å		c =
		α = 90°		β = 105.82°		γ

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	4.44

To enter the database, simply click on one of the tabs above.



a	5.5	2.95	3.03
b	1.00	1.00	0.90
c	50	50	40
d			
e			
f			
g			
h			
i			
j			
k			
l			
m			
n			
o			
p			
q			
r			
s			
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aa			
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dd			
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rr			
ss			
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vv			
ww			
xx			
yy			
zz			
aaa			
bbb			
ccc			
ddd			
eee			
fff			
ggg			
hhh			
iii			
jjj			
kkk			
lll			
mmm			
nnn			
ooo			
ppp			
qqq			
rrr			
sss			
ttt			
uuu			
vvv			
www			
xxx			
yyy			
zzz			
aaa			
bbb			
ccc			
ddd			
eee			
fff			
ggg			
hhh			
iii			
jjj			
kkk			
lll			
mmm			
nnn			
ooo			
ppp			
qqq			
rrr			
sss			
ttt			
uuu			
vvv			
www			
xxx			
yyy			
zzz			

Crystallographic Open Database

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

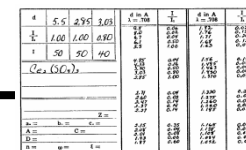


222319 entries



- contain either a CIF

All data on this site have been placed in the public domain by the contributors.





01-20-2009

Crystallography Open Database

(Output limited to 300 entries maximum, see the [hints and tips](#))

Note: substructure search by SMARTS is currently available in a subset of COD containing 40 000 structures

 s Donators	 CIF file	<div> <div>COD ID: 9007497</div> <div> Formula: - Cu₂ O - Comments: Kurfel, 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; </div> </div>





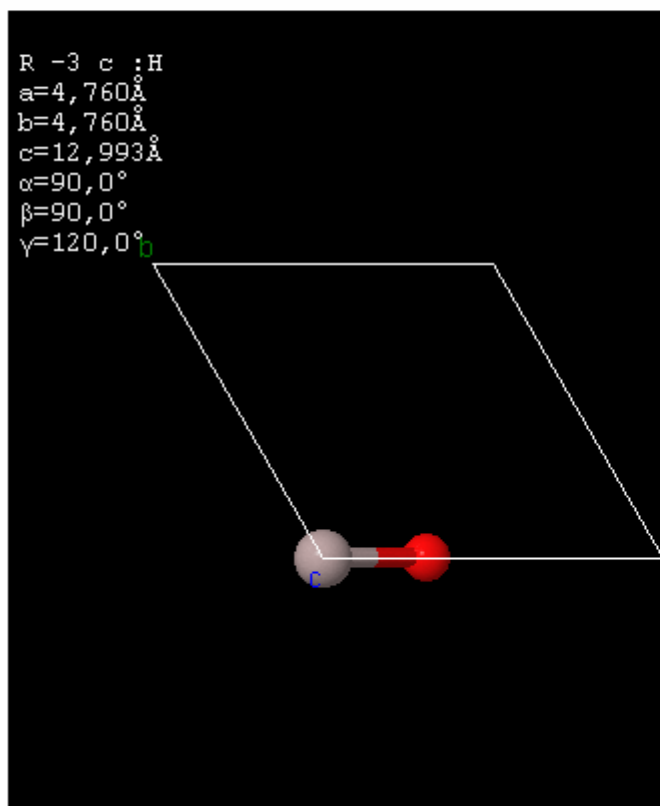
a	b	c	α	β	γ	V	Z	ρ	ρ_c
4.760	4.760	12.993	90	90	120	254.977	2	3.59	3.59
$\frac{1}{a}$	$\frac{1}{b}$	$\frac{1}{c}$	$\frac{1}{\alpha}$	$\frac{1}{\beta}$	$\frac{1}{\gamma}$	$\frac{1}{V}$	$\frac{1}{Z}$	$\frac{1}{\rho}$	$\frac{1}{\rho_c}$
0.210	0.210	0.077	1.097	1.097	0.833	0.00392	0.5	0.279	0.279
$\frac{1}{a^2}$	$\frac{1}{b^2}$	$\frac{1}{c^2}$	$\frac{1}{\alpha^2}$	$\frac{1}{\beta^2}$	$\frac{1}{\gamma^2}$	$\frac{1}{V^2}$	$\frac{1}{Z^2}$	$\frac{1}{\rho^2}$	$\frac{1}{\rho_c^2}$
0.0441	0.0441	0.0060	1.192	1.192	0.694	0.00154	0.25	0.077	0.077
$\frac{1}{a^3}$	$\frac{1}{b^3}$	$\frac{1}{c^3}$	$\frac{1}{\alpha^3}$	$\frac{1}{\beta^3}$	$\frac{1}{\gamma^3}$	$\frac{1}{V^3}$	$\frac{1}{Z^3}$	$\frac{1}{\rho^3}$	$\frac{1}{\rho_c^3}$
0.0093	0.0093	0.0005	1.301	1.301	0.462	0.00016	0.125	0.037	0.037

CIF Information Card

Information card for 9007496

[9007495](#) << **9007496** >> [9007497](#)

Preview



Structure parameters

Common name	Corundum
Formula	- Al ₂ O ₃ -
Calculated formula	- Al ₁₂ O ₁₈ -
Title of publication	Electric field gradients and charge density in corundum alpha-Al ₂ O ₃
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