

PHASE IDENTIFICATION AND SEARCH/MATCH

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- Lachlan Cranswick
- Pamela Whitfield
- Nicola Döbelin
- Bussaraporn Patarachao

Special acknowledgments to:

- Mati Raudsepp
- Lee Groat and Julie (Melluish) McIntosh who started me on this XRD journey



INTRODUCTION

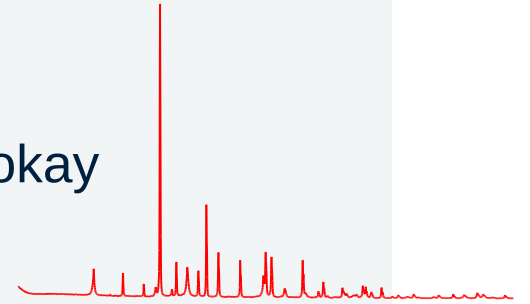


THE PROCESS OF PHASE IDENTIFICATION



What do we need?

- **Data:** acquire data for the purpose of phase ID – qualitative quality is okay
 - What do you do with it? How do you look at it?
- **Software for phase ID:** commercial, freeware; spreadsheet plot
 - Not absolutely necessary but it definitely helps
- **Database** ('fingerprints'): commercial database, free database, books, individual files
 - Historically, phase identification was done manually (Hanawalt, Fink methods)



SEARCH/MATCH



- From the DIFFRAC.EVA User Manual (DOC-M88-EXX200 V2 – 09.2011)

“The Aim of EVA Search/Match

The purpose of EVA Search/Match is to search the current scan of an **unknown** material and then identify **reference patterns** that are likely to explain the unknown scan. A Search algorithm is applied, comparing the reference patterns of a database to the scan. The algorithm gives a rank to the Patterns and lists the "best candidates". The user must compare the pattern to the scan and accept or reject the found pattern. This is called the match procedure.”

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BEFORE WE CONTINUE



Software and Databases shown and used in this presentation:

Software:

- EVA and Apex (Bruker)
- HighScorePlus (Malvern-Panalytical)
- QualX (Institute of Crystallography-CNR) – free for academic and non-profit

Databases:

- PDF-2 from the International Centre for Diffraction Data (ICDD)
- Crystallography Open Database (COD)
- American Mineralogist Crystal Structure Database (AMCSD)

DATABASES AND RESOURCES



- Inorganic and organic **databases** and crystal structure **resources**:

- PDF-5+, PDF-4 Minerals, PDF-4 Axiom and PDF-2 (Powder Diffraction File) from the **ICDD** (International Center for Diffraction Data) – commercial
- **ICSD** (Inorganic Crystal Structure Database) – commercial
- COD (Crystallography Open Database) – open access
- **AMCSD** (American Mineralogist Crystal Structure Database) – open access
- CSD (Cambridge Structural Database; organic and organometallic) – commercial

- for phase identification
- no atomic positions given so can't use for Rietveld work

- Published papers
- Unpublished data: your files; research group files – create your own database; personal communication

➤ CIF file → convert to diffraction pattern then bring it into the phase ID software to try to **match**

- For more information on databases: see International Tables for Crystallography (2019). Vol. H Chapter 3.7, pp. 304-324 (Crystallographic databases and powder diffraction by James Kaduk)

DATABASE EXAMPLE

You can search databases to find crystal structures and their information – but this is not the matching process...

... what do you need for matching?

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database focused on minerals and solids of interest to mineralogists.

For questions about AMCSDB, please [Contact Us](#).

Mineral

Pyrite

Author

Includes:

Chemistry

S, Fe

Excludes:

Cell Parameters and Symmetry

Diffraction Search

General Search

Display

amc long form

amc short form

SEARCH

RESET



Pyrite

Mineral Name

Pyrite

AMC File Contents

Pyrite
Ramsdell L S
American Mineralogist 10 (1925)
The crystal structures of some
Locality: natural, unknown
_database_code_amcsd 0000006
5.38 5.38 5.38 90 90 90 Pa3
atom x y z
Fe 0 0 0
S .338 .338 .338

AMC File

Pyrite_0000006.amc

Minimal CIF

Pyrite_0000006.cif

Record 2* - Click here to view

afef1092228a3d59

Mineral Name

Pyrite

AMC File Contents

Pyrite
Bayliss P
American Mineralogist 62 (1977) 1168-1172
Crystal structure refinement of a weakly anisotropic pyrite
cubic model
_database_code_amcsd 0000605
5.4166 5.4166 5.4166 90 90 90 Pa3
atom x y z Biso
Fe 0 0 0 .28
S .3851 .3851 .3851 .33

AMC File

Pyrite_0000605.amc

Minimal CIF

Pyrite_0000605.cif

Original CIF

No Files Uploaded

DIF File

Pyrite_0000605.dif

Bayliss P (1977) Crystal structure refinement of a weakly anisotropic pyrite. American Mineralogist 62, 1168-1172 [view file]

Record 3* - Click here to view

c8b7a207025a714ac040b9e113c1

Mineral Name

Pyrite

Ideal IMA Formula

FeS₂

AMC File Contents

Pyrite
Bayliss P
American Mineralogist 62 (1977) 1168-1172
Crystal structure refinement of a weakly anisotropic pyrite
_database_code_amcsd 0000606
5.4166 5.4166 5.4166 90 90 90 P1
atom x y z B(1,1) B(2,2) B(3,3) B(1,2) B(1,3) B(2,3)
Fe1 .0010 .0020 .0030 .0023 .0024 .0017 .0000 .0000 .0004
Fe2 .4966 .0001 .5036 .0026 .0026 .0019 .0002 -.0003 -.0001
Fe3 .5001 .5020 .0011 .0026 .0021 .0022 .0007 -.0002 -.0003
Fe4 -.0006 .5013 .5038 .0026 .0026 .0016 .0001 -.0002 -.0001
S1 .3857 .3832 .3840 .0020 .0018 .0004 -.0007 -.0003 -.0004
S2 .1149 .6114 .8846 .0038 .0069 .0050 .0002 -.0001 -.0007
S3 .8854 .1157 .6143 .0034 .0001 -.0002 -.0001 -.0004 -.0004
S4 .6153 .8865 .1141 .0039 .0075 .0039 -.0003 -.0008 -.0010
S5 .6151 .6132 .6137 .0035 .0046 .0049 .0002 -.0002 -.0000
S6 .8854 .3818 .1149 .0026 -.0005 -.0002 .0000 -.0003 .0002
S7 .1147 .8856 .3841 .0035 .0057 .0054 .0001 -.0003 -.0001
S8 .3857 .1161 .8842 .0014 -.0004 .0011 .0004 .0001 .0004

global

ical_name_mineral 'Pyrite'

author_name

iss P'

nal_name_full 'American Mineralogist'

nal_volume 62

nal_year 1977

nal_page_first 1168

nal_page_last 1172

section_title

tal structure refinement of a weakly anisotropic pyrite

c model

base_code_amcsd 0000605

ical_formula_sum 'Fe S2'

length_a 5.4166

length_b 5.4166

length_c 5.4166

angle_alpha 90

angle_beta 90

angle_gamma 90

volume 158.921

l_crystal_density_diffrn 5.015

symmetry_space_group_name_H-M 'P a 3'

loop_

_space_group_symop_operation_xyz

'x,y,z'

'1/2+z,x,1/2-y'

'z,1/2-x,1/2+y'

'1/2-z,1/2+x,y'

'-z,-x,-y'

'1/2+y,1/2-z,-x'

'1/2-y,-z,1/2+x'

'-y,1/2+z,1/2-x'

'y,z,x'

'x,1/2-y,1/2+z'

'1/2-x,1/2+y,z'

'1/2+x,y,1/2-z'

'-x,-y,-z'

'1/2-z,-x,1/2+y'

'-z,1/2+x,1/2-y'

'1/2+z,1/2-x,-y'

'z,x,y'

'1/2-y,1/2+z,x'

'1/2+y,z,1/2-x'

'y,1/2-z,1/2+x'

'-y,-z,-x'

'-x,1/2+y,1/2-z'

'1/2+x,1/2-y,-z'

'1/2-x,-y,1/2+z'

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

Fe 0.00000 0.00000 0.00000 0.00355

S 0.38510 0.38510 0.38510 0.00418

REMEMBER DIFFRACTION

Crystalline materials have long range periodicity. Once you know the crystal structure of a material you can generate a list of expected diffraction peaks (peak positions/d-spacings with relative intensities) and this is like a **fingerprint** of the material. It is unique to the material although there may be similar diffraction patterns across similarly structured materials.

X-ray diffraction experiment: An X-ray beam interacts with a crystalline substance and diffraction occurs when the Bragg equation is satisfied resulting in a set of diffraction peaks. These peaks are characterized by peak positions (related to d-spacings), intensities, and peak shape.

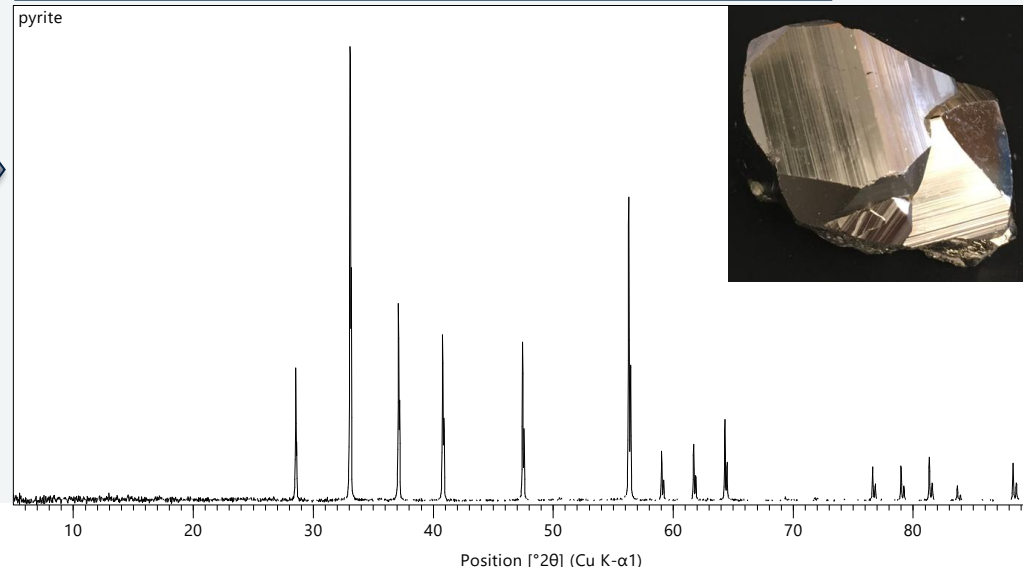
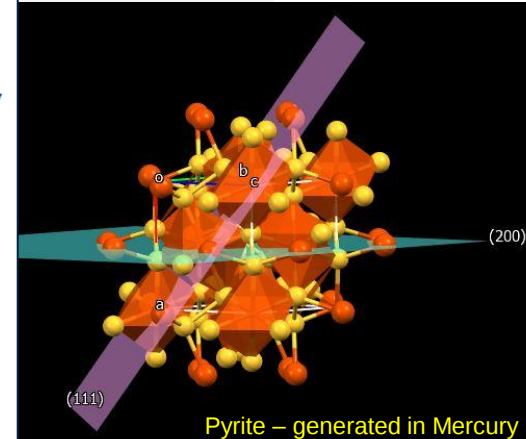
$$n\lambda = 2d\sin\theta \quad \text{Bragg equation}$$

Pyrite
Bayliss P
American Mineralogist 62 (1977) 1168-1172
Crystal structure refinement of a weakly anisotropic pyrite
cubic model
_database_code_amcsd 0000605

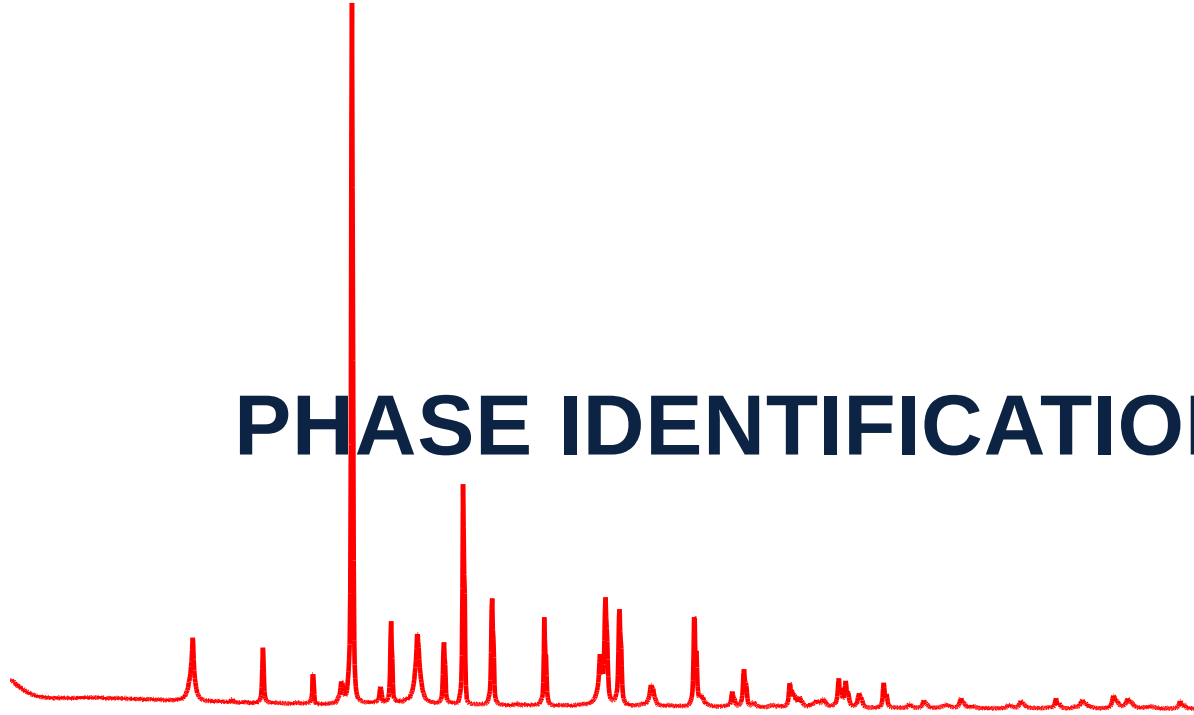
CELL PARAMETERS: 5.4166 5.4166 5.4166 90.000 90.000 90.000
SPACE GROUP: Pa3
X-RAY WAVELENGTH: 1.541838
Cell Volume: 158.921
Density (g/cm3): 5.014
MAX. ABS. INTENSITY / VOLUME**2: 47.22399758
RIR: 3.067
RIR based on corundum from Acta Crystallographica A38 (1982) 733-739

2-THETA	INTENSITY	D-SPACING	H	K	L	Multiplicity
28.54	39.18	3.1273	1	1	1	8
33.08	95.52	2.7083	2	0	0	6
37.11	54.86	2.4224	2	1	0	12
40.81	45.47	2.2113	2	1	1	24
47.48	51.01	1.9151	2	2	0	12
56.33	100.00	1.6332	3	1	1	24
59.08	15.84	1.5636	2	2	2	8
61.75	16.11	1.5023	3	0	2	12
64.35	15.90	1.4476	3	2	1	24
64.35	5.65	1.4476	3	1	2	24
76.69	10.49	1.2427	3	3	1	24
79.06	6.56	1.2112	4	2	0	12
79.06	6.56	1.2112	4	0	2	12
81.42	8.55	1.1820	4	2	1	24
83.76	4.21	1.1548	3	3	2	24
88.41	12.51	1.1057	4	2	2	24

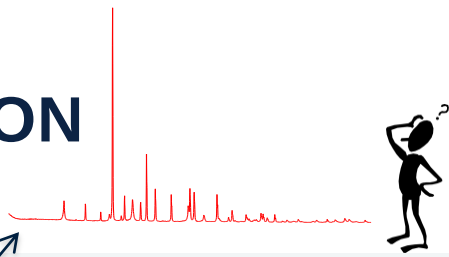
XPOW Copyright 1993 Bob Downs, Ranjini Swaminathan and Kurt Bartelmehs
reference, see Downs et al. (1993) American Mineralogist 78, 1104-1107.



PHASE IDENTIFICATION

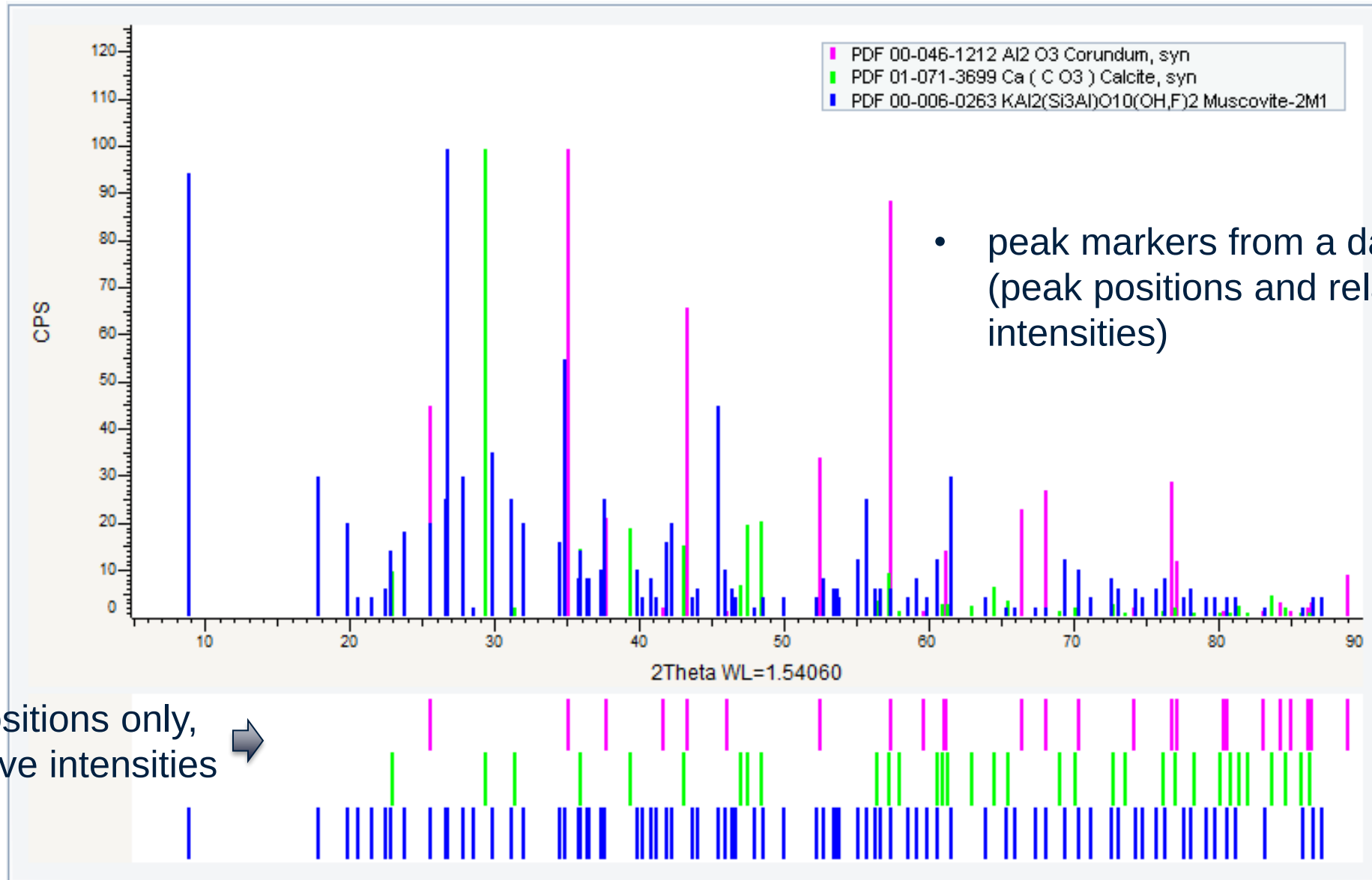


PHASE IDENTIFICATION

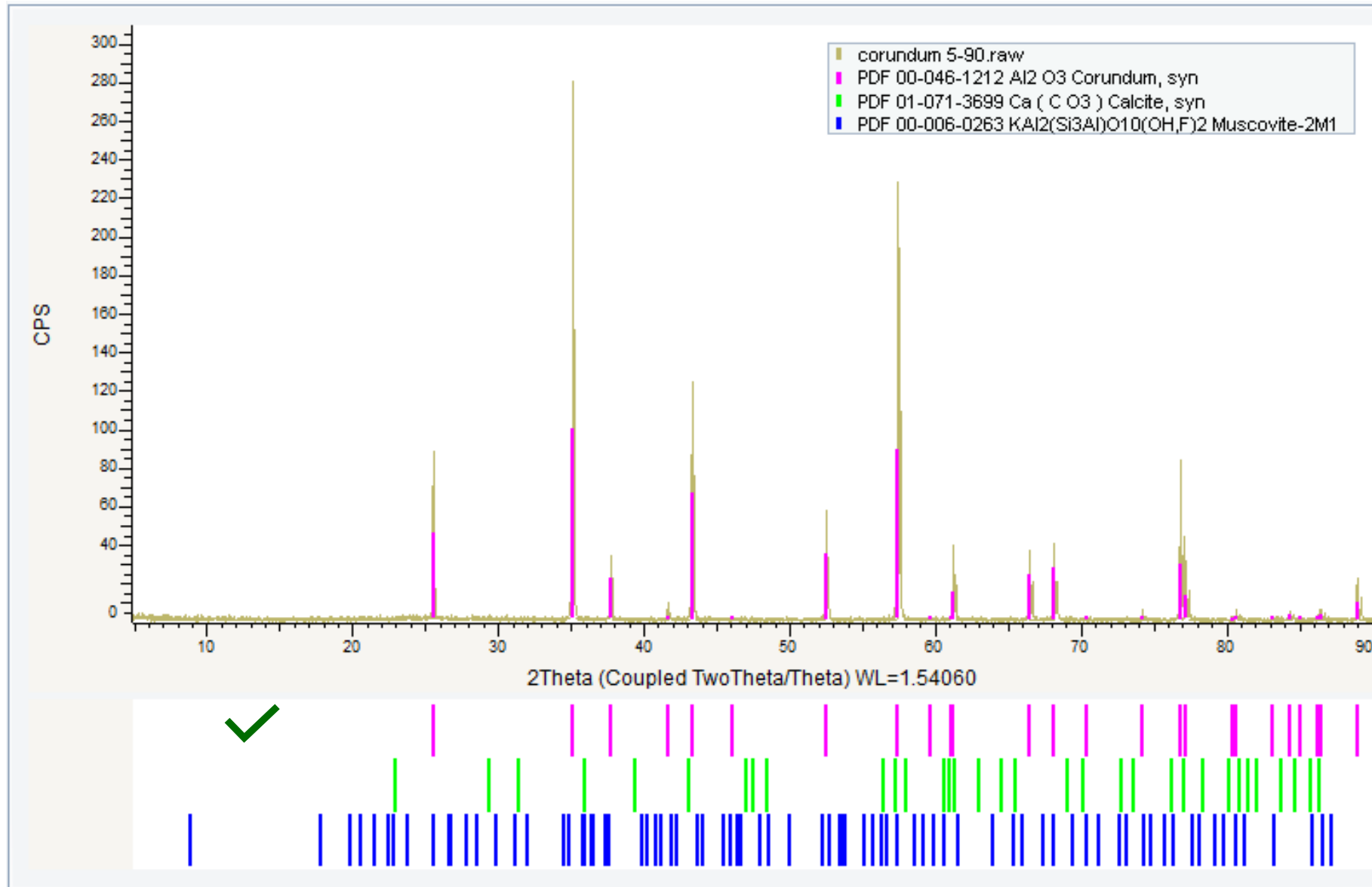


- It's like matching a fingerprint to known patterns in a database
- Peak positions are key for phase identification
 - Relative intensities are helpful but we know that the peak intensities may differ from ideal
- XRD is sensitive to the crystalline structure of the material (not directly sensitive to the elemental chemistry); the chemistry of your phase should be confirmed by other means
 - chemical analyses and sample information help with phase identification
- Note: you need to do phase identification before you attempt to try quantitative phase analysis (QPA)

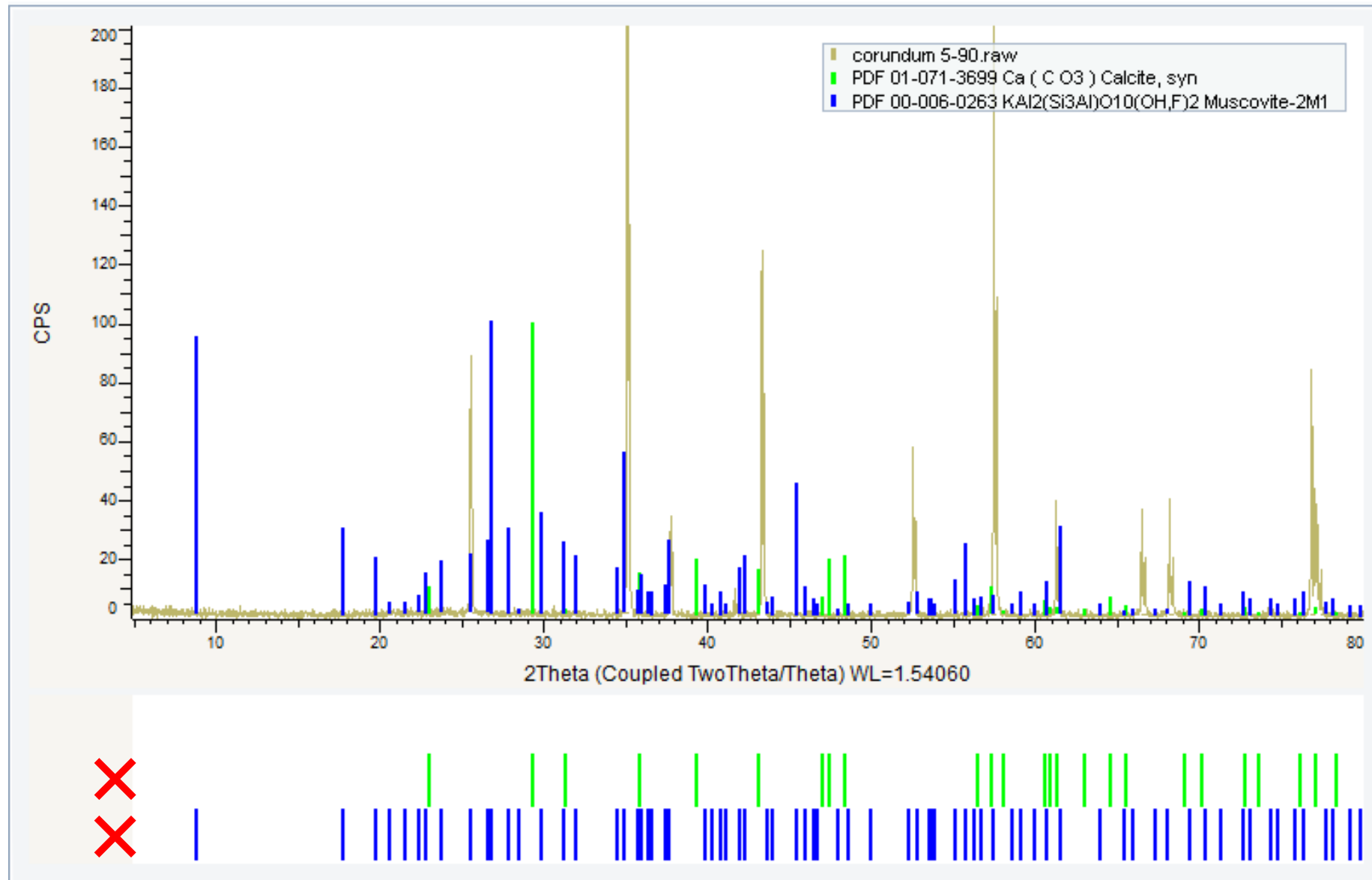
FINGERPRINT



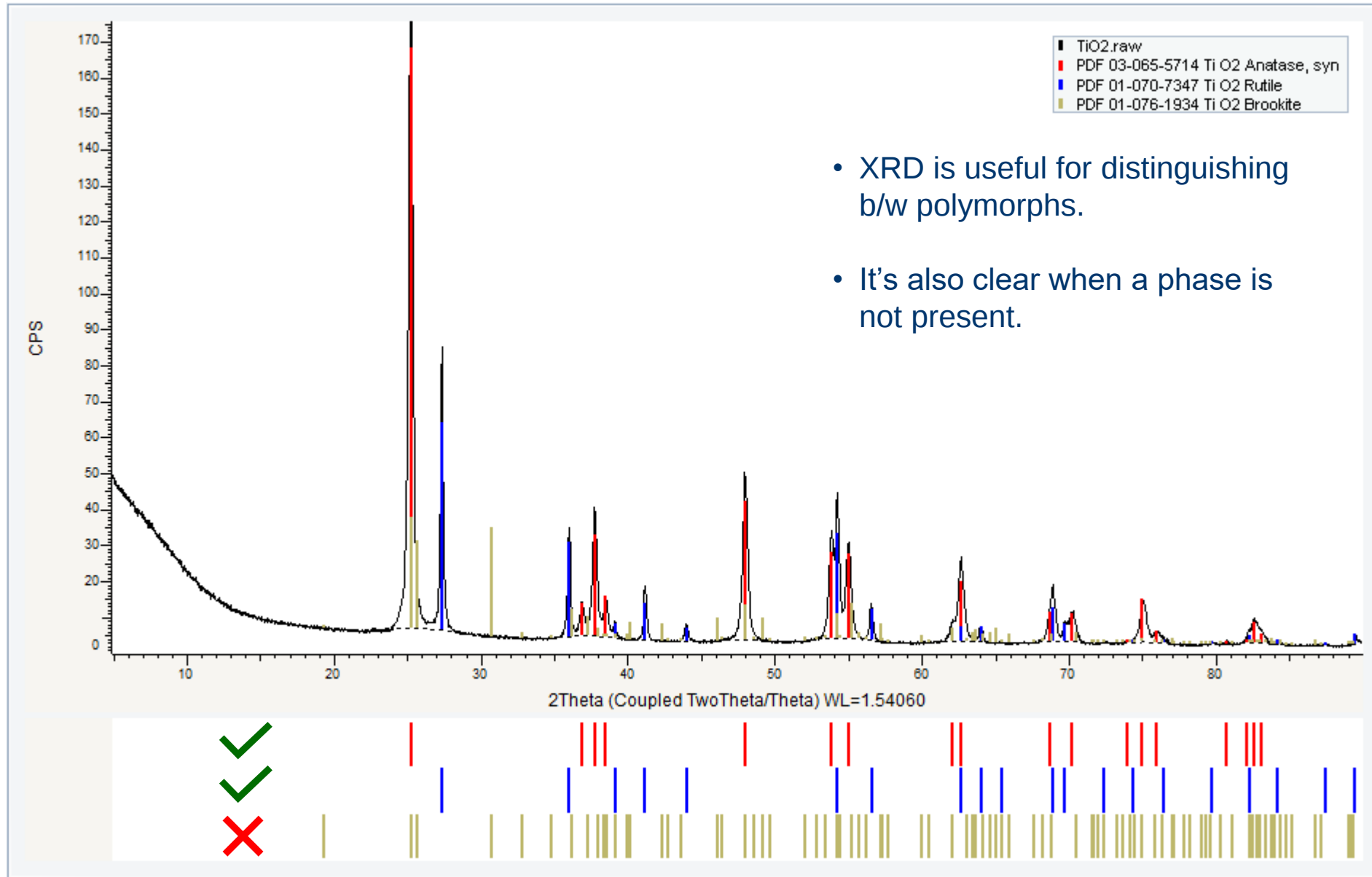
Match! – it is the set of peaks that make up the fingerprint of the pattern. You need to match the set not just one peak.



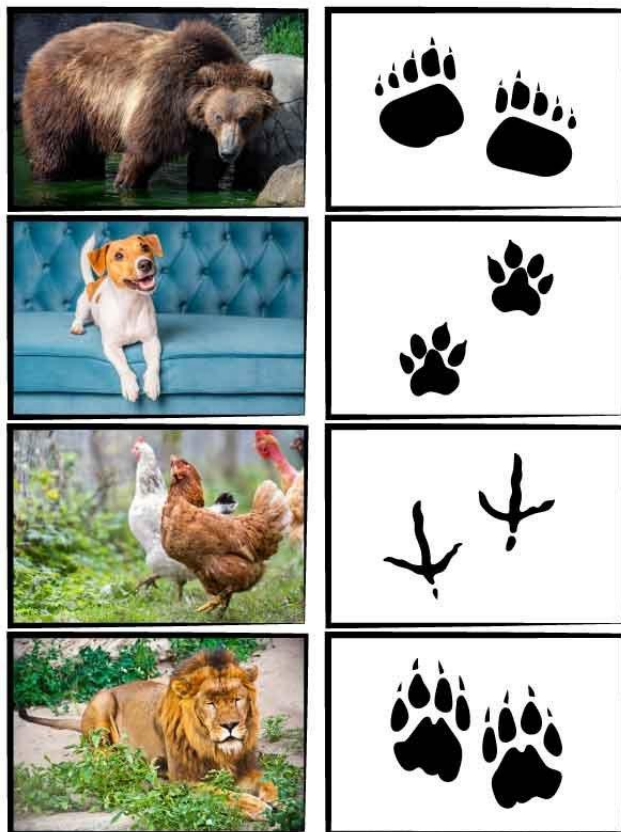
NOT a match! – it is the set of peaks that make up the fingerprint of the pattern. You need to match the set not just one peak. The absence of peaks should also match.



POLYMORPH EXAMPLE



- XRD is useful for distinguishing b/w polymorphs.
- It's also clear when a phase is not present.



MATCH

SEARCH/MATCH



- Search results are dependant on criteria input by the user
- Search results are suggestions or candidates
 - It is up to the researcher to select the most likely matches
 - Automatic match function in the software can be helpful but the software has no idea if the match that it selected is correct or not – that is up to you!
- An interactive process between the user and the software + database
 - User knowledge, experience, and intuition are valuable to the process

Get to work! Start practising and gaining experience!

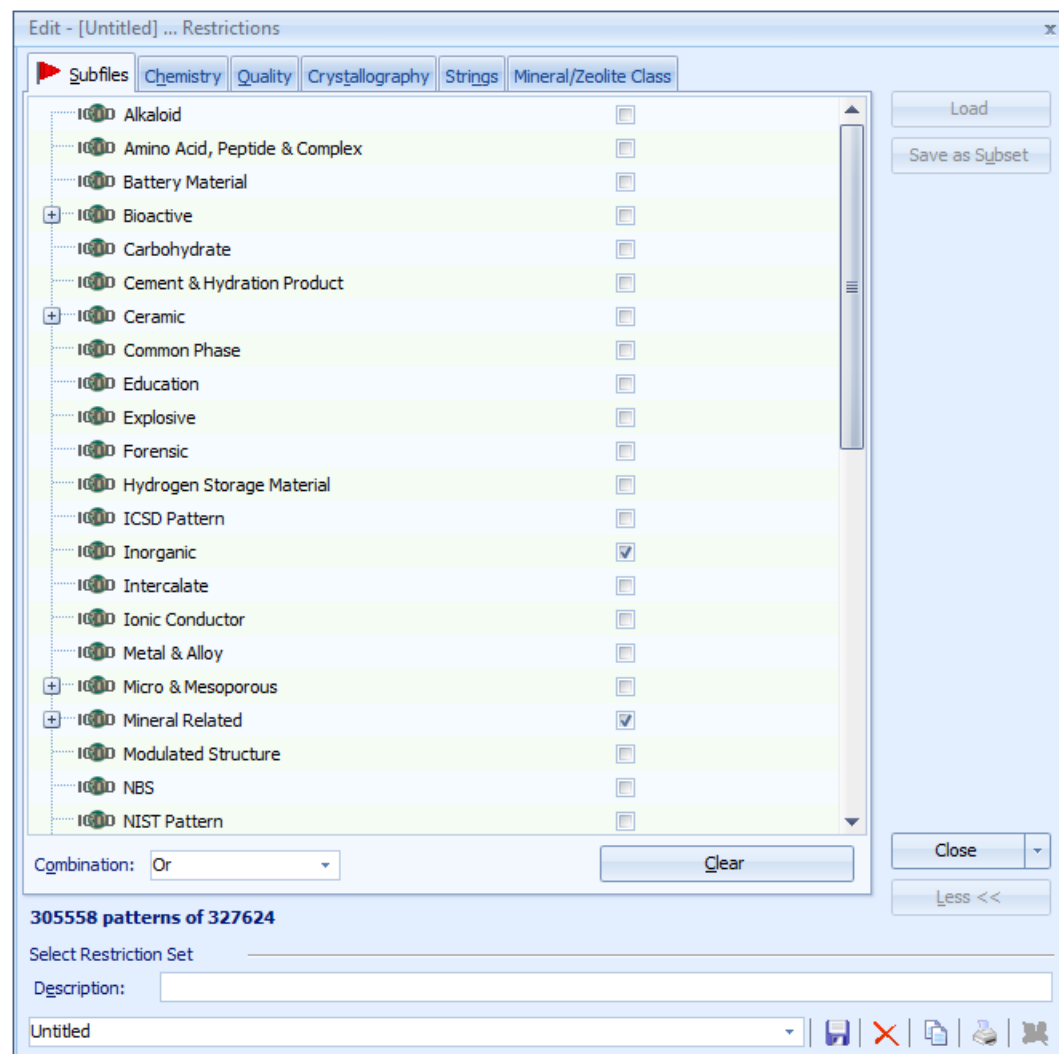
SEARCH/MATCH – SAMPLE INFORMATION



- Obtain as much information as possible about the sample
 - Where did it come from? What is likely to be in it? What are the reaction conditions? etc.
 - What industry is it from? – geological, cement, pharmaceutical, battery, etc.
 - Tip: useful to learn the language of the industry
 - Are there any chemical analyses available?
 - I usually ask the client to list **every possible element** in the system including anything the sample came into contact with such as the reaction vessel, atmosphere, wash solution, etc.
 - Have a sample with no information? – start with a light/common element search with the mineral database in the hope that it is a common substance
 - Minerals are naturally occurring crystalline materials and many are common substances (with a common name that's easy to recognize)
 - If you get stuck, go back to the client and ask for more information.

SEARCH – NARROWING THE FIELD

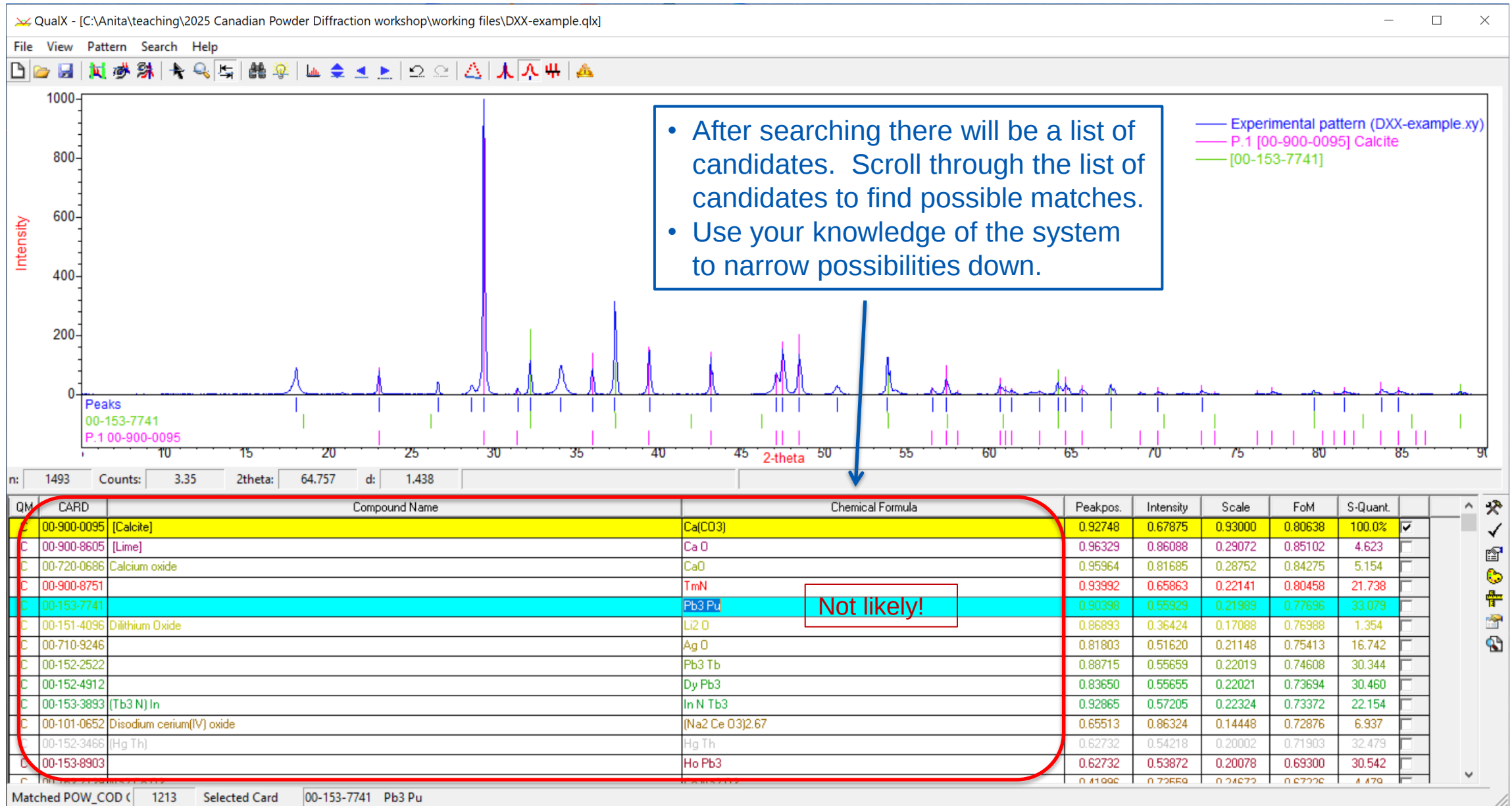
Database Subfiles:



Database Filter unknown .raw #2		
PDF-2 2026		
Auto Rebuild Click to filter Candidates Clear		
* Share		
Filter	Value	Candidates
☒ Full Files		
☐ Dual		1491
☒ Inorganic		312013
☐ Organic		55770
☐ Subfiles		
☐ Strunz Mineral Classification		27812
☐ Zeolite		4971
☒ Meas. Conditions		
☒ Ambient		310849
☐ Non ambient		58425
☐ Temperature		48414
☐ Temperature and Pressure		1161
☐ Pressure		8850
☐ Quality Marks		
☒ Status		
☒ Primary		280745
☐ Deleted		21530
☒ Alternate		66995
☐ Colors		
☐ Sources		
☐ Element # in Formula		369274
☐ Density		369274
☐ Crystallographic Data		
☐ SQ Analysis		



MATCHING



SEARCHING – POSSIBLE ELEMENTS



Periodic Table

- Grey – possible elements
- Red – excluded elements
- Green – has to be there
- Blue – one of the elements has to be there

• A light element search

The image displays two screenshots of a software interface titled "Chemical Filter unknown .raw #1". The interface includes a dropdown menu set to "PDF-2 2026", buttons for "Auto", "Rebuild", "Click to filter Candidates", and "Clear". Below these are checkboxes for "D", "A", "M", and "N", followed by "Import", "Export", and "Share" options.

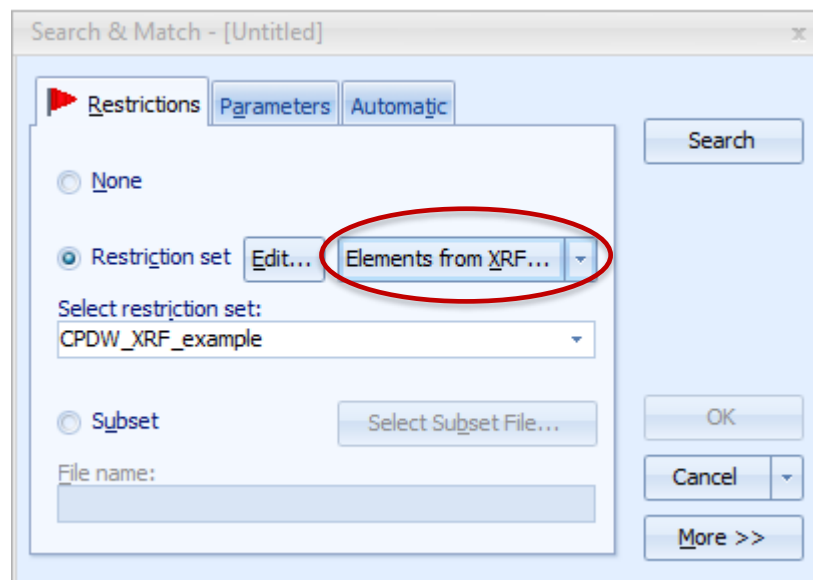
The top screenshot shows a periodic table where only Hydrogen (H) and Helium (He) are highlighted in red, while all other elements are grey. The bottom screenshot shows a more extensive search, with many elements highlighted in red, including those in the p-block, d-block, and f-block (lanthanides and actinides). The legend on the left indicates that grey represents possible elements, red represents excluded elements, green represents elements that must be present, and blue represents elements that must be present.

SEARCHING – CHEMICAL ANALYSES

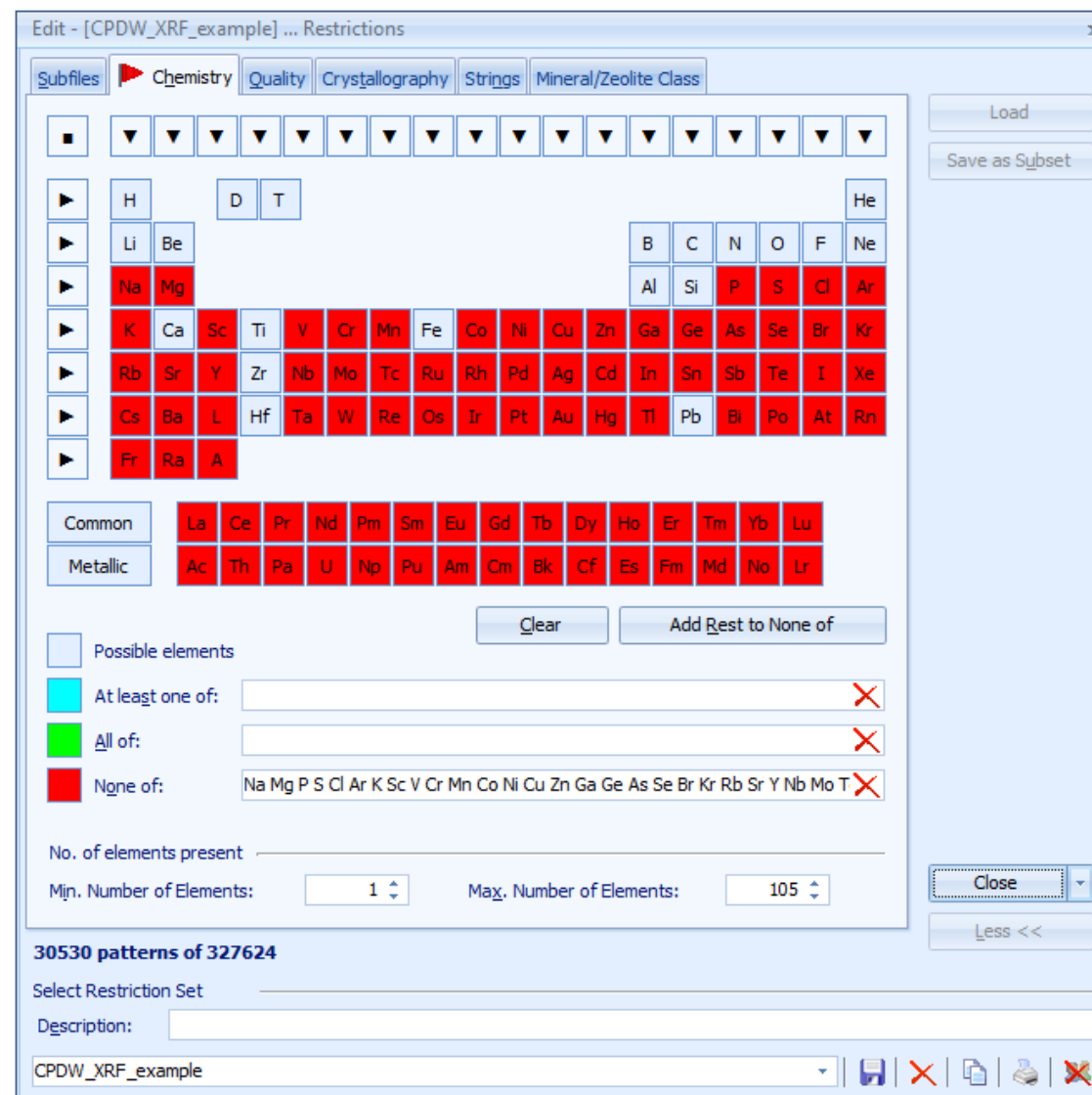


XRF results

- Grey – possible elements
- Red – excluded elements



- This allows you to search only the elements known to be in your system.



SEARCHING – ELEMENT SPECIFIC



Element focused

- Grey – possible elements
- Red – excluded elements
- Green – has to be there

Chemical Filter unknown .raw #2

PDF-2 2026

Auto Rebuild Click to filter Candidates Clear

D A M N * Share

H D T He

Li Be B C N O F Ne

Na Mg Al Si P S Cl Ar

K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr

Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe

Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn

Fr Ra Ac

Lanthanides / Actinides

Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Ln

Searching for a copper phase

Searching for an oxide

Formula

- (NH₄)₂(Cu(H₂O)₆)(SO₄)₂
- CuO·3H₂O
- Cu_{0.4}V₂O₅
- Cu₆Al(SO₄)(OH)₁₂Cl(H₂O)₃
- Cu_{1.94}Zn_{0.06}V₂O₇
- Cu₂V₂O₇
- Na₄(Cu₄O₂(SO₄)₄)(Na_{0.26}Cu_{0.37})Cl
- Cu_{1.3}V₉O₂₂
- Cu₂(NO₃)(OH)₃
- Cu_{1.9}Zn_{0.1}V₂O₇
- Zn₇Cu₄(O₄H₇)_{0.3}(OH)₁₃((SiO(OH)₃)_{0.7}(SO₄))
- Cu₆(Al_{0.94}Fe_{0.06})(SO₄)(OH)₁₂Cl(H₂O)₃
- MgCu(Mg_{0.74}Cu_{0.26})(PO₄)₂(H₂O)
- Na_{9.74}Cu_{11.40}O₂₅I₀
- Cu₇PS₆
- (Zn,Cu)₇(SO₄)₂(OH)₁₀·3H₂O
- Ca₃₀Al₃₈Cu₂₅
- CuCu₂(OH)₃Cl₂
- (Zn₅Cu)₂Zn₂(OH)₁₃((S_{0.5}Si_{0.5})(O_{2.5}(OH)_{1.5}))₂
- Cu₄(SO₄)(OH)₆(H₂O)

Formula

- KZn(SO₄)Cl
- Na₃V(Si₄O₁₁)(H₂O)
- KBe(PO₃(OH))F
- Na_{3.98}(MnO₂)₁₃
- Na₂Fe₂V(PO₄)₃
- Ca₂(Al_{2.684}Sc_{0.316})Si₃O₁₂(OH)
- Na_{7.4}Al_{6.4}Si_{25.6}O₆₄·O₂₀
- NaZn(H₂PO₃)₃(H₂O)
- K₂Fe(PO_{2.5}F_{1.5})₂F₂
- Na_{3.94}(MnO₂)₁₃
- CaB₃O₃(OH)₅(H₂O)
- Li(NH₄)₂B₃P₄O₁₆
- Na₂(CO₃)H₂O
- KV(PO₄)O
- HFe₄(CO)₁₂BH₂
- KMnV₂O₆Cl(H₂O)₂
- Ca₂(Al_{2.63}Sc_{0.37})Si₃O₁₂(OH)
- Mg_{0.735}Zn_{2.265}(PO₄)₂(H₂O)₄
- Na₆Mn(SO₄)₄
- Ca(HPO₄)

SEARCHING – ELEMENT SPECIFIC

Element focussed

- Grey – possible elements
- Red – excluded elements
- Green – has to be there
- Blue – one of the elements has to be there

▶	H		D	T															He
▶	Li	Be									B	C	N	O	F				Ne
▶	Na	Mg									Al	Si	P	S	Cl				Ar
▶	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
▶	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
▶	Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
▶	Fr	Ra	A																
Common				La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
Metallic				Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

No.	Ref. Code	Chemical Formula
1	ICDD 01-082-1460	Rb Fe (Se O4)2
2	ICDD 00-068-0618	Sr Ca Ni Te O6
3	ICDD 01-085-7056	Sr3 Fe2 Te O9
4	ICDD 01-084-8465	Sr Ca Ni Te O6
5	ICDD 01-075-8547	Sr2 Fe1.33 Te0.67 O6
6	ICDD 01-075-8546	Sr2 Fe1.33 Te0.67 O6
7	ICDD 01-075-8548	Sr2 Fe1.33 Te0.67 O6
8	ICDD 01-075-8549	Sr2 Fe1.33 Te0.67 O6
9	ICDD 01-089-8379	Sr2 Cu (Te O6)
10	ICDD 01-072-4327	Cd2 (Te2 O7)
11	ICDD 00-050-0401	Cu Sr2 Te O6
12	ICDD 01-075-9489	Sr2 ((Fe1.33 Te0.67) O6)
13	ICDD 00-047-0010	Sc2 Te4 O11
14	ICDD 01-080-8053	Sr4 (V O2)2 (Se O3)4 (Se2 O5)
15	ICDD 01-083-3020	Se Mn O3
16	ICDD 01-076-3289	Sr2 Fe1.47 Te0.53 O6
17	ICDD 01-077-5338	Ag4 (Mo2 O5) (Se O4)2 (Se O3)
18	ICDD 00-055-0529	Cd2 Te2 O7
19	ICDD 01-077-5586	Cd4 V2 Te3 O15
20	ICDD 01-070-0241	Mn (Se O3)
21	ICDD 00-031-0830	Mn Se O3
22	ICDD 00-036-0881	Ca Te O3
23	ICDD 01-072-7832	Mn (Se O3)
24	ICDD 01-085-2142	Ca3 Fe2 (Se O3)6
25	ICDD 01-086-9658	Cu2 (Se O3) F2
26	ICDD 01-076-9766	Sr (Te3 O8)
27	ICDD 00-053-0208	Sr2 Fe1.33 Te0.67 O6
28	ICDD 00-029-0897	Sr2 Mn Te O6
29	ICDD 01-082-3425	Y6 Te O12
30	ICDD 01-072-7831	(Cu0.25 Mn0.75) (Se O3)



These are just a few examples – the search criteria should be tailored to your samples.

SEARCHING – CHEMICAL FILTER



Element focussed

- Grey – possible elements
- Red – excluded elements
- Green – has to be there
- Blue – one of the elements has to be there

Search using common elements – all blue is okay

Common

Metallic

Clear

Add Rest to None of

Possible elements

At least one of: H Li B C N O F Na Mg Al Si P S Cl K Ca Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se X

All of: X

None of: He Be Ne Ar Sc Kr Rb Y Tc Ru Rh Pd Te Xe Cs La Ce Pr Nd Pm Sm Eu Gd Tb D X

SEARCHING – CHEMICAL FILTER



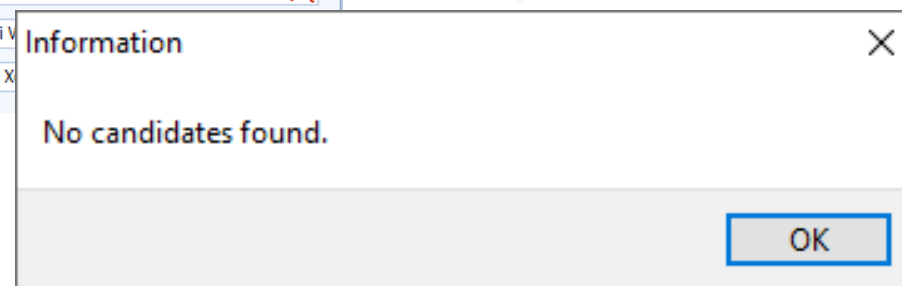
Element focussed

- Grey – possible elements
- Red – excluded elements
- Green – has to be there
- Blue – one of the elements has to be there

Don't do this.....Why?

The screenshot shows a chemical filter interface with a periodic table. Elements are colored: grey for possible, red for excluded, and green for required. The 'None of' filter box is selected, and a yellow arrow points from it to an 'Information' dialog box.

Filter	Elements
Possible elements	
At least one of:	
All of:	H Li B C N O F Na Mg Al Si P S Cl K Ca Ti V
None of:	He Be Ne Ar Sc Kr Rb Y Tc Ru Rh Pd Te Xe



SEARCHING – CHEMICAL FILTERS



Some built-in filters are available or you can create your own.

Element focussed

- Grey – possible elements
- Red – excluded elements
- Green – has to be there
- Blue – one of the elements has to be there

The screenshot shows a web application titled "Chemical Filter unknown .raw #2". It features a search bar with "PDF-2 2026" and buttons for "Auto", "Rebuild", "Click to filter Candidates", and "Clear". Below the search bar, there are four colored squares (D, A, M, N) and a filter menu with "Import", "Export", and "Rock Forming Minerals" (which is circled in red). A blue arrow points from the text "Some built-in filters are available or you can create your own." to the "Rock Forming Minerals" filter. The main area displays a periodic table with elements colored according to the filter: Grey (possible), Red (excluded), Green (must be there), and Blue (one must be there). The "Rock Forming Minerals" filter highlights elements like H, Li, Na, K, Rb, Cs, Fr, D, T, Be, Mg, Ca, Sr, Ba, Ra, Ac, Ti, Zr, Hf, Ta, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Pb, Bi, Po, At, Rn, and the Lanthanides/Actinides series.

SEARCHING – BY NAME OR FILE NUMBER



Search List		
	Name	Formula
1	Calcite	CCaO3
2	Calcite	CCaO3
	calcite	CCaO3
	Magnesium calcite	CCa0.94Mg0.06O3
	Calcite, magnesian	CCa0.9Mg0.1O3
	Calcite	CCaO3
	Calcite	CCa0.9Mg0.1O3
	Calcite	CCaO3
	Calcite	CCaO3
	Calcite	CCaO3
	Calcite	CCaO3
	Calcite	CCaO3
14	Calcite	CCa0.936Mg0.064O3
15	Calcite	CCa0.871Mg0.129O3
16	Calcite	CCaO3
17	Calcite	CCaO3
18	Calcite	CCaO3
19	Calcite	CCaO3
20	Calcite	CCaO3
21	Calcite	CCaO3

Search / Match DXX-example.raw #1

Databases Match Lists **Names** Options

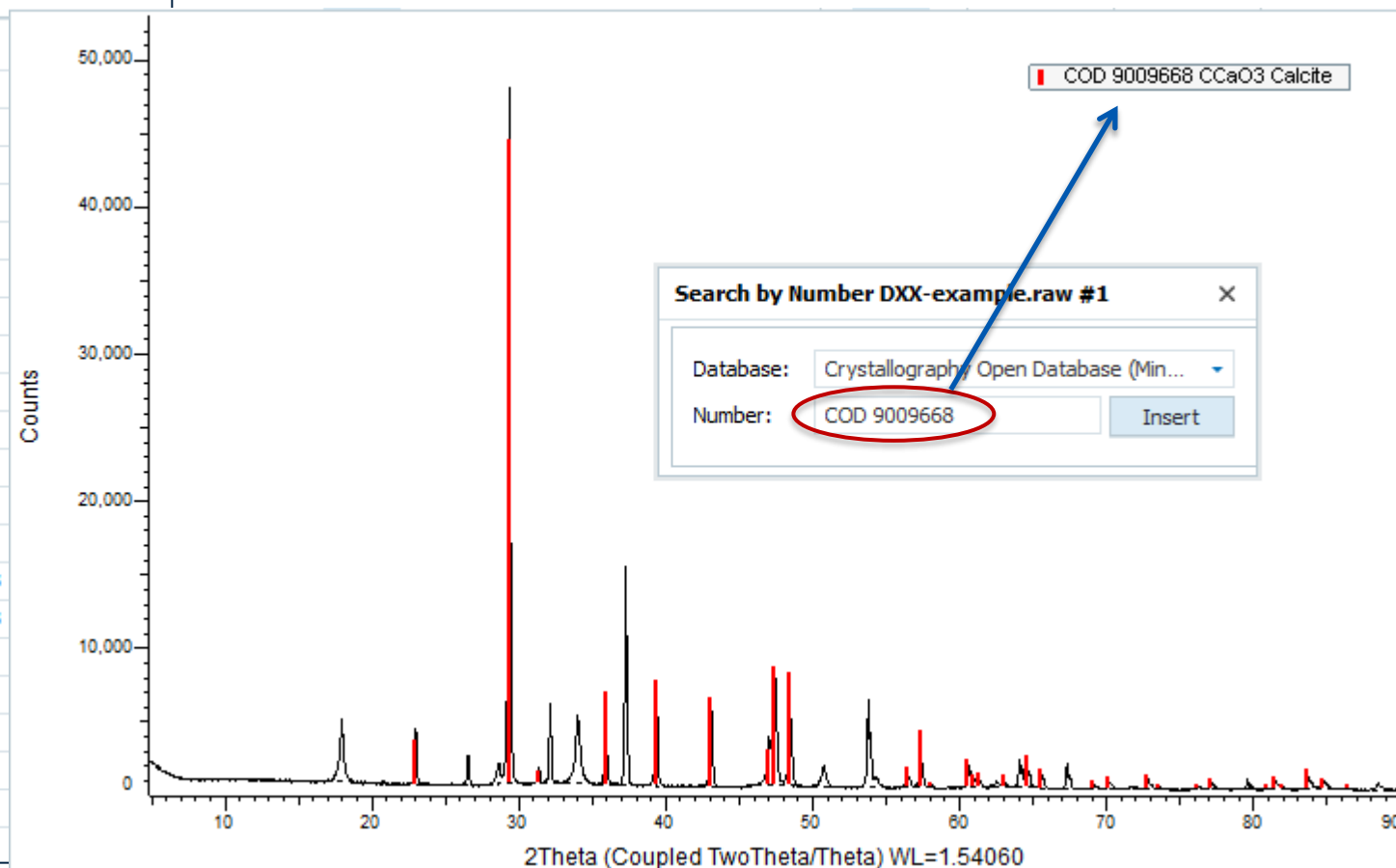
calcite

Use Filters ☐

And ☒ Or ☐

ABC Name

Use ? and * for partial names e.g. BO*HMIT?, parenthesis for authors e.g. (BOGUE), curly brackets for formulas e.g. {CaCO3}, dash to negate the result e.g. QUARTZ -BETA



SEARCHING – BY CRYSTALLOGRAPHY



Edit - [Untitled] ... Restrictions

Subfiles Chemistry Quality **Crystallography** Strings Mineral/Zelite Class

Min Max Min Max

a [Å]: 5.405 5.415 Density [g/cm³]:

b [Å]: 5.405 5.415 No. of Formula Units (Z):

c [Å]: 5.405 5.415 Reference Intensity Ratio:

alpha [°]: Cell Volume [Å³]:

beta [°]: Space Group Number:

gamma [°]:

ratio a/c: Crystal System: Cubic

Min - Max

Value - Deviation [%]

Clear

Close

Less <<

148 patterns of 327624

Select Restriction Set

Description:

Untitled

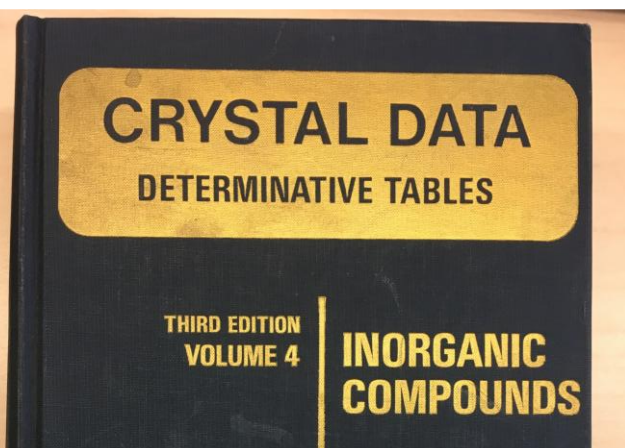
Candidates: Search

No.	Ref. Code	Cryst. Syst.	Space Gr...	Cell	Compound Name
1	ICDD 03-065-2974	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Nickel Silicon
2	ICDD 00-047-1655	Cubic	F-43m	a 5.407 - b 5.407 - c 5.407	Cobalt Zinc Sulfide
3	ICDD 00-016-0576	Cubic	F-43m	a 5.405 - b 5.405 - c 5.405	Strontium Arsenic Sulfide
4	ICDD 01-085-8588	Cubic	F-43m	a 5.406 - b 5.406 - c 5.406	Zinc Sulfide
5	ICDD 01-081-5205	Cubic	F-43m	a 5.410 - b 5.410 - c 5.410	Copper Sulfide
6	ICDD 01-071-5971	Cubic	F-43m	a 5.409 - b 5.409 - c 5.409	Zinc Sulfide
7	ICDD 01-073-8755	Cubic	F-43m	a 5.409 - b 5.409 - c 5.409	Nickel Zinc Sulfide
8	ICDD 03-065-4586	Cubic	F-43m	a 5.409 - b 5.409 - c 5.409	Nickel Zinc Sulfide
9	ICDD 03-065-9585	Cubic	F-43m	a 5.409 - b 5.409 - c 5.409	Zinc Sulfide
10	ICDD 01-071-4258	Cubic	F-43m	a 5.407 - b 5.407 - c 5.407	Cobalt Iron Zinc Sulfide
11	ICDD 01-078-2500	Cubic	Fd-3m	a 5.406 - b 5.406 - c 5.406	Silicon
12	ICDD 01-072-2669	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Nickel Zinc
13	ICDD 03-065-9470	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Nickel Zinc
14	ICDD 00-050-0202	Cubic	Fm-3m	a 5.413 - b 5.413 - c 5.413	Cerium Gadolinium Yttrium ...
15	ICDD 01-080-6505	Cubic	Fm-3m	a 5.405 - b 5.405 - c 5.405	Calcium Cerium Oxide
16	ICDD 03-065-7441	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Manganese Zinc Sulfide
17	ICDD 00-027-0843	Cubic		a 5.410 - b 5.410 - c 5.410	Neodymium Antimony Oxide
18	ICDD 01-081-9692	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Cerium Yttrium Oxide
19	ICDD 01-080-6915	Cubic	Fm-3m	a 5.405 - b 5.405 - c 5.405	Cerium Oxide
20	ICDD 01-080-5532	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Cerium Yttrium Oxide
21	ICDD 01-073-2568	Cubic	F-43m	a 5.406 - b 5.406 - c 5.406	Zinc Sulfide
22	ICDD 01-082-9831	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Cerium Oxide
23	ICDD 01-075-0167	Cubic	Fm-3m	a 5.405 - b 5.405 - c 5.405	Dysprosium Cerium Oxide
24	ICDD 01-089-4958	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Manganese Zinc Sulfide
25	ICDD 01-074-6110	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Zinc Sulfide
26	ICDD 03-065-1691	Cubic	F-43m	a 5.411 - b 5.411 - c 5.411	Zinc Sulfide
27	ICDD 01-081-9649	Cubic	F-43m	a 5.409 - b 5.409 - c 5.409	Molybdenum Phosphide
28	ICDD 01-071-6544	Cubic	F-43m	a 5.412 - b 5.412 - c 5.412	Zinc Iron Sulfide
29	ICDD 01-083-5829	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Cerium Praseodymium Oxide
30	ICDD 01-080-4831	Cubic	Fm-3m	a 5.406 - b 5.406 - c 5.406	Cerium Praseodymium Oxide

SEARCHING – BY UNIT CELL



- an aside: (single crystal) users sometimes do phase ID by checking the unit cell



ORTHORHOMBIC

a/b	c/b	a
0.5729	0.5437	9.81

Past – used
cell ratios

Cordierite
17.127±21, 9.812±6, 9.312±3)bac. From B1S
aggregates. Light blue. Opt. neg.: 1.554

Information card for entry 2300571

[2300570](#) << [2300571](#) >> [2300572](#)

Preview

HM: P 21 21 21 #19
a=5.963Å
b=9.042Å
c=18.401Å
α=90.000°
β=90.000°
γ=90.000°

Coordinates [2300571.cif](#)
Structure factors [2300571.hkl](#)
Original paper (by DOI) [HTML](#)

Unit Cell:
a= 5.96Å, α=90.00°, V=993Å³
b= 9.05Å, β=90.00°, Orthorhombic P
c=18.39Å, γ=90.00°

Formula	a [Å]	b [Å]	c [Å]	α [°]	β [°]	γ [°]	Space G
None	5.97	9.04	18.41	90.00	90.00	90.00	P 21 21
C12 H10 O2 S	5.96	9.01	18.38	90.00	90.00	90.00	P 21 21
C12 H10 O2 S	5.96	9.03	18.39	90.00	90.00	90.00	P 21 21
C12 H10 O2 S	5.96	9.04	18.40	90.00	90.00	90.00	P 21 21
C12 H10 O2 S	5.96	9.05	18.38	90.00	90.00	90.00	P 21 21
C12 H10 O2 S	5.97	9.04	18.39	90.00	90.00	90.00	P 21 21
C31 H11 O2 S	5.97	9.05	18.41	90.00	90.00	90.00	P 21 21
C11 H10 O2 S	5.97	9.04	18.41	90.00	90.00	90.00	P 21 21
C11 H10 O2 S	5.97	9.04	18.41	90.00	90.00	90.00	P 21 21
C11 H10 O2 S	5.96	9.04	18.40	90.00	90.00	90.00	P 21 21
C11 H10 O2 S	5.96	9.04	18.40	90.00	90.00	90.00	P 21 21
C23 H30 N2 O2	18.54	6.06	8.94	90.00	90.00	90.00	P 21 21
C10 H12 O2 S	6.01	9.03	18.15	90.00	90.00	90.00	P 21 21
C10 H7 N2 O2	8.81	18.36	5.86	90.00	90.00	90.00	P 21 21
C6 H2 N8 O4	5.72	8.81	18.60	90.00	91.55	90.00	P 1 21/d

Elements Filter:

☐ Only These Elements

Databases

Database	Count	Created
APEX DB	25	2019-11-19
CSD	21	2019-11-19
COD	3	2022-12-19
local CIF/RES	8	2025-07-09

Locate Structure

Automatic Mode

Start at: Collect Data

Stop after: Search

Run

Manual Mode

☒ Collect Data

☒ Harvest Spots

☒ Index

☐ Domains

☒ Bravais

☐ Refine

☒ Search

Unit cells:

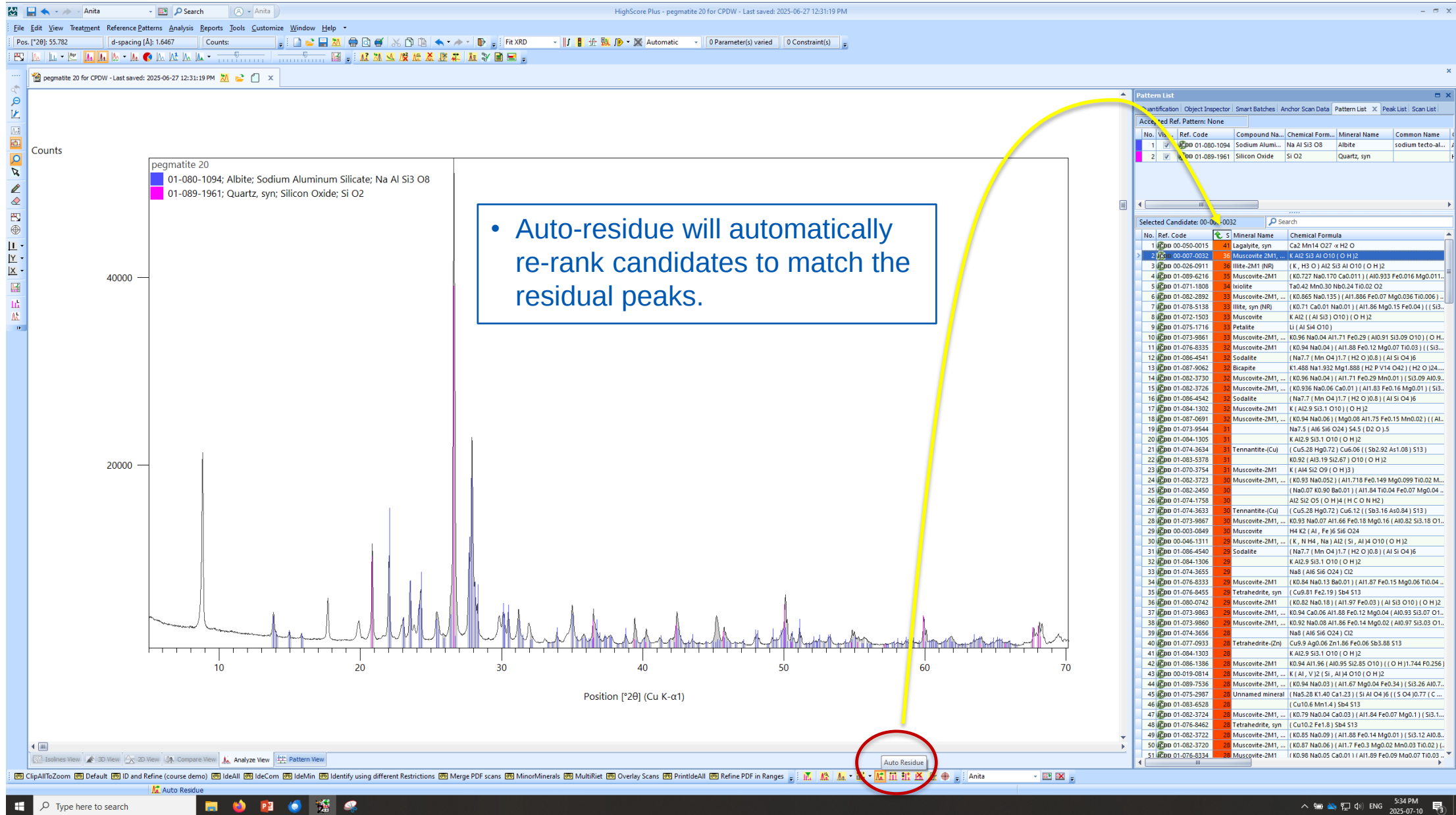
a= 5.96Å, α=90.00°, V=993Å³
b= 9.05Å, β=90.00°, Orthorhombic P
c=18.39Å, γ=90.00°

Reflections:

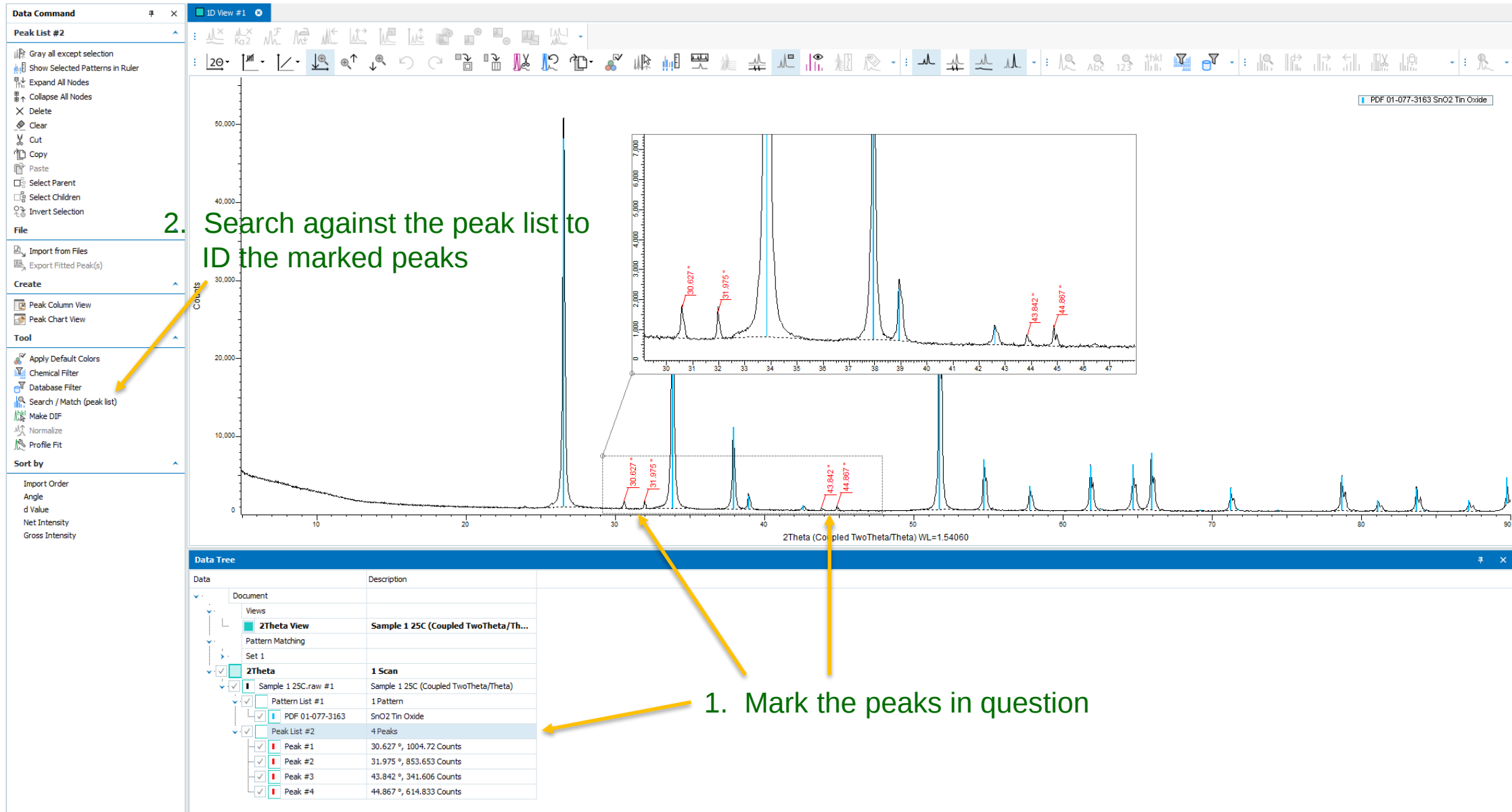
Group 0: 78 reflections

Present – search unit cell

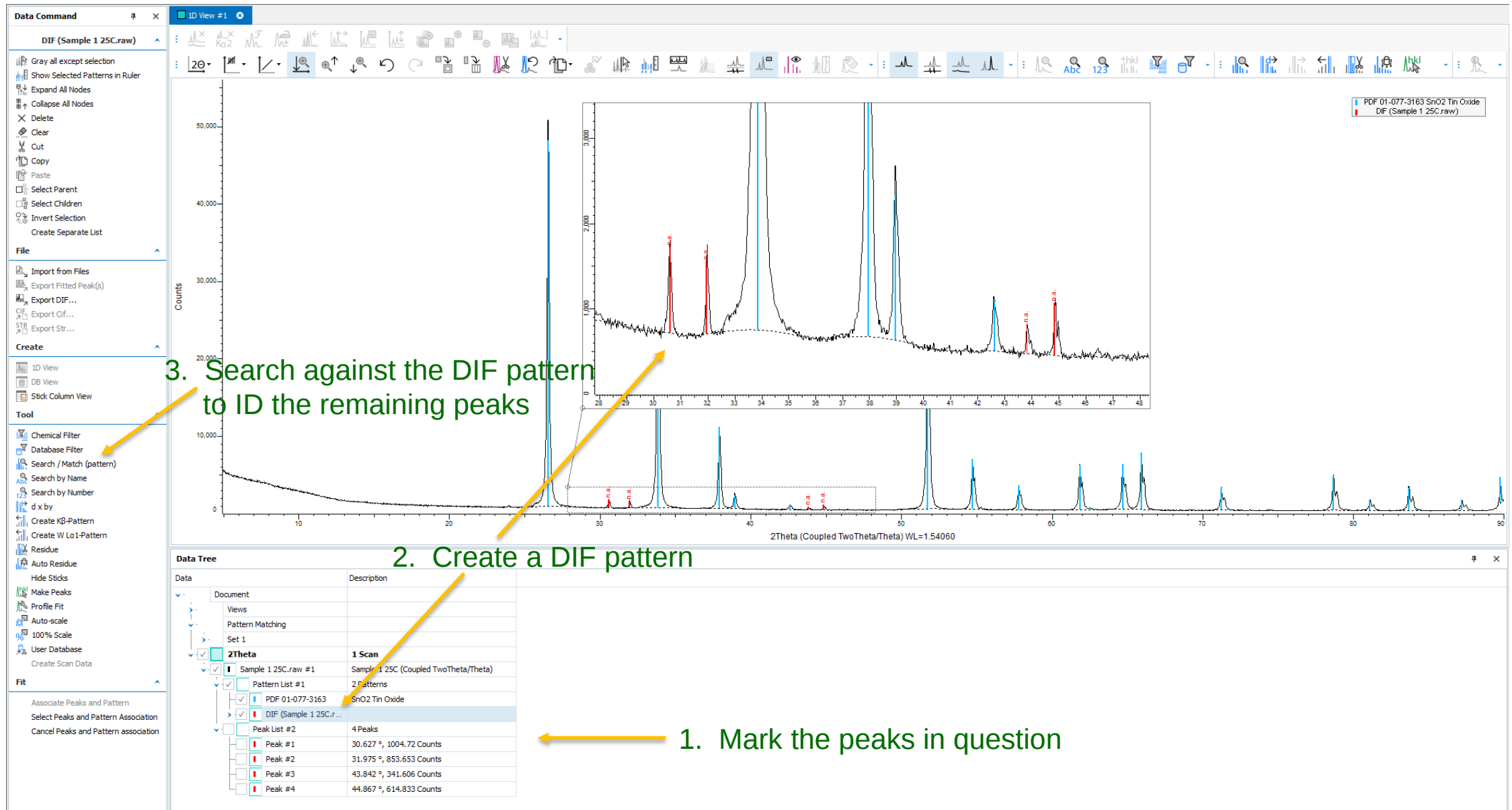
SEARCHING – RESIDUAL PEAKS



SEARCHING – SPECIFIED PEAKS



SEARCHING – SPECIFIED PEAKS, DIF PATTERN



STILL HAVING TROUBLE?

OTHER TIPS AND TRICKS



CHANGE DATABASES



- Sometimes a pattern or clue to the unidentified phase might be in a different database

Manage Databases

Database Name	Use	Database Location	Content Type	Prope...	Convert	Writable	Data
ICDD PANalytical Example Database	☐	C:\Users\User\Documents\PANalytical\HighScore\Example	PDF-2 flat file	...	...		HighS
ICDD PDF-2 2026	☐	PDF2026	PDF-2 RDB	...	...		Sybas
ICDD PDF-2 2026	☐	C:\Program Files\ICDD PDF-2 Release 2026\PDF-2 2026.hs	PDF-2 RDB	...			HighS
COD24_HS4x	☐	C:\Databases\COD24_HS4x.hsrdb	Converted CIF files	...			HighS
CSD Database, The Cambridge Crystallographic ...	☒	C:\Databases\CSD_2025_2_Database.hsrdb	CSD Database	...			HighS

Total Number of Patterns: 1297328

CSD Da...25-600 1297328

Disk Usage

0 179.159358 318537.477716 636895.7951,074.95
Gigabyte

Add HighScore Database... Search for databases Create new empty database... Convert OK Cancel

EVA Settings

General Decimal Places Database DB Patterns Filters XRF Fit Colors Sp

Search / Match Databases

- ☒ Enable "Deleted" PDF Patterns
- ☐ Enable "Hypothetical" PDF Patterns
- ☒ Enable "Alternate" PDF Patterns
- ☒ Auto-Search Results as Candidates
- ☐ Remember Auto-Search state

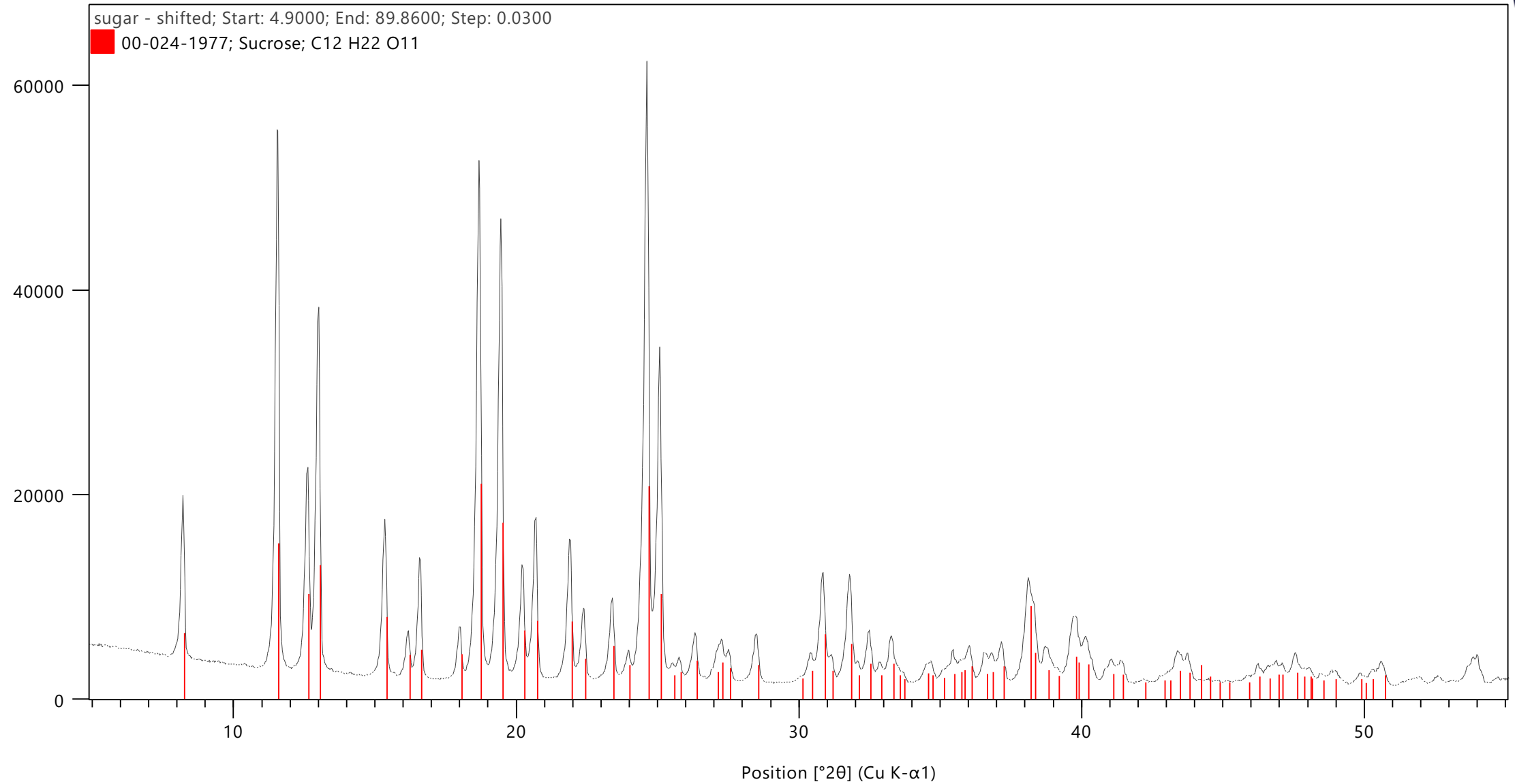
Default Databases

- ☐ Crystallography Open Database (Full) (rev.294853)
- ☐ Crystallography Open Database (Minerals) (rev.294865)
- ☒ PDF-2 2026

PEAK SHIFTS (see next slide)



Counts



PEAK SHIFTS (see previous slide)



Search & Match - [Untitled]

Restrictions Parameters Automatic

Data source: Peak Data

Scoring scheme: ☒ Single phase ☐ Multi phase

☐ Auto residue ☐ Demote unmatched strong

☐ Match intensity ☐ Allow pattern shift

Known Two Theta shift [°2θ]: 0.000

Search

Candidates:

No.	Ref. Code	S	Compound Name	Chemical Formula
1	ICDD 00-062-1061	50	Diaquo 1,4-bis(imidazol-1-...	Co (H ₂ O) ₂ (N ₂ C ₃ H ₃) C ₆ H ₄
2	ICDD 01-082-5942	48	Curium Oxide Sulfide	Cm ₁₀ O S ₁₄
3	ICDD 01-076-9357	48	Calcium Mercury	Ca ₉ Hg ₅₄ (Ca _{1.92} Hg _{0.08})
4	ICDD 01-085-1407	48	Sodium Calcium Iron Vana...	(Na _{0.7} Ca _{0.3}) (V _{7.6} Fe _{0.4}) O ₂
5	ICDD 01-086-6420	48	Mercury Ytterbium	Yb ₁₁ Hg ₅₄
6	ICDD 01-070-5161	48	Thallium Tin Fluoride	(Tl ₅ F ₃) (Sn F ₆)
7	ICDD 01-081-6277	47	Mercury Ytterbium	Yb ₁₄ Hg ₅₁
8	ICDD 01-087-2745	46	Barium Zinc Iron Oxide	Ba ₆ Zn ₅ Fe ₄₂ O ₇₄
9	ICDD 01-071-1187	46	Bromine Antimony Fluoride	(Br F ₂) (Sb F ₆)
10	ICDD 00-053-0122	46	Cadmium Chloride Thiourea	C ₂ H ₈ CdCl ₂ N ₄ S ₂
11	ICDD 00-069-1141	46	Lithium glycolate monohy...	C ₂ H ₃ LiO ₃ ·H ₂ O
12	ICDD 00-070-1030	45	4,5-Dihydroxy-1-phenethyl...	C ₁₁ H ₁₄ N ₂ O ₃
13	ICDD 01-085-9599	45	Cesium Hydrogen Sulfate ...	Cs ₃ (H S O ₄) ₂ (H ₂ P O ₄)
14	ICDD 01-085-3221	45	Cesium Hydrogen Sulfate ...	Cs ₃ (H S O ₄) ₂ (H ₂ P O ₄)
15	ICDD 01-082-4378	45	Barium Mercury Zinc	Ba Hg _{3.40} Zn _{0.60}
16	ICDD 01-087-1598	44	Potassium Hydrogen Germ...	K ₃ H (Ge ₇ O ₁₆) (H ₂ O) _{3.137}
17	ICDD 00-041-1368	44	Calcium Manganese Silicate	Ca Mn ₁₄ + ₃ SiO ₂₄
18	ICDD 00-070-0293	43	Silver Zinc Iron Molybdate	Ag Zn ₃ Fe (Mo O ₄) ₅
19	ICDD 03-065-1166	43	Erbium Germanium Nickel	Er Ge ₂ Ni ₃
20	ICDD 01-076-9694	43	Tin Gallium Indium Titaniu...	Ga _{3.18} In _{0.82} Sn _{2.7} Ti _{0.3} O ₁₂
21	ICDD 01-073-0898	43	Tin Oxide Hydroxide Phos...	Sn ₃ O (OH) (P O ₄)
22	ICDD 01-076-1846	43	Calcium Silicate	Ca (Si O ₃)
23	ICDD 00-069-0886	43	Naphthalene	C ₁₀ H ₈
24	ICDD 01-083-0495	43	Potassium Zinc Deuteride	K ₃ (Zn D ₅)

• not selected

Allow pattern shift

Search & Match - [Untitled]

Restrictions Parameters Automatic

Data source: Peak Data

Scoring scheme: ☒ Single phase ☐ Multi phase

☐ Auto residue ☐ Demote unmatched strong

☐ Match intensity ☐ Allow pattern shift

Known Two Theta shift [°2θ]: 0.000

Search

Candidates:

sucrose

• no candidates found

Search & Match - [Untitled]

Restrictions Parameters Automatic

Data source: Peak Data

Scoring scheme: ☒ Single phase ☐ Multi phase

☐ Auto residue ☐ Demote unmatched strong

☐ Match intensity ☒ Allow pattern shift

Known Two Theta shift [°2θ]: 0.000

Search

Candidates:

sucrose

47 ICDD 00-024-1977 40 Sucrose C₁₂H₂₂O₁₁

• selected; redo search

• Allowing a pattern shift brought sucrose into the candidate list

PEAK SHIFTS (see previous slide)



Search / Match DIF (sugar shifted.raw)

Matched 259051 / 260302 Candidates in 2.8 s.

Databases

Match Lists

Names

Options

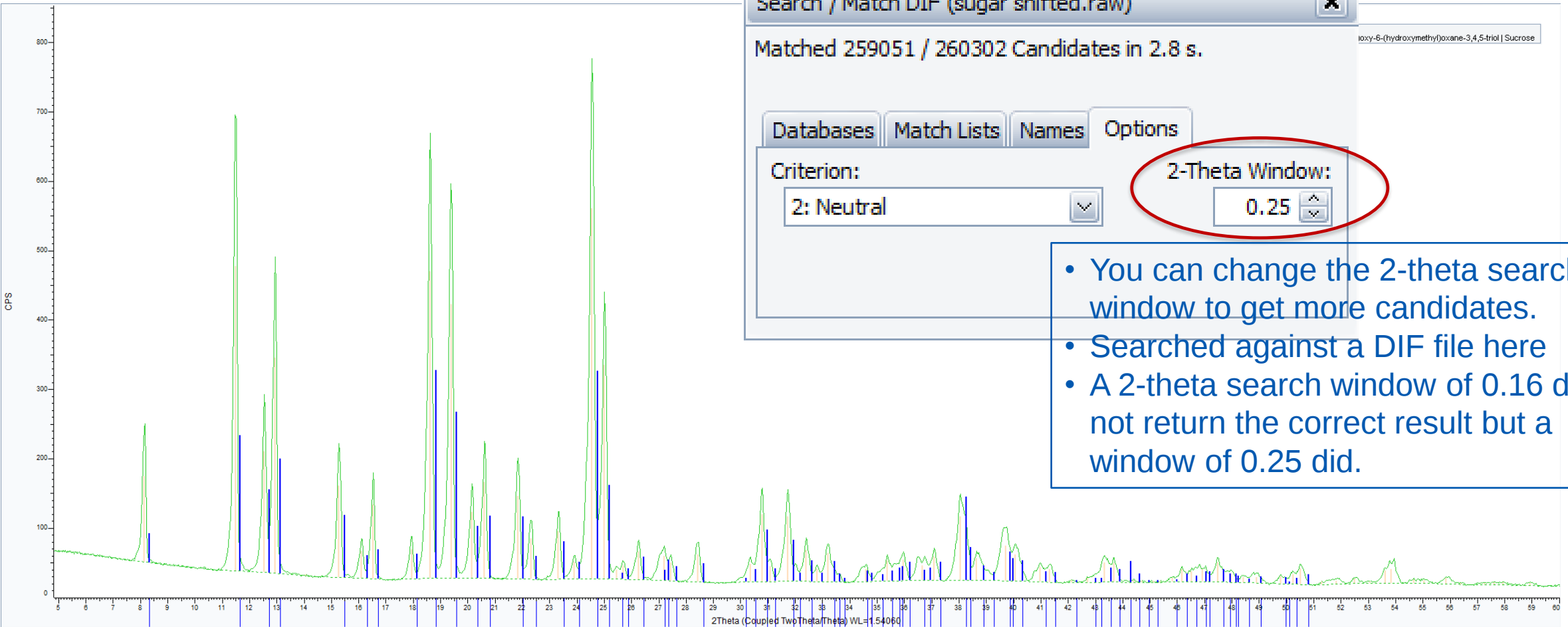
Criterion:

2: Neutral

2-Theta Window:

0.25

- You can change the 2-theta search window to get more candidates.
- Searched against a DIF file here
- A 2-theta search window of 0.16 did not return the correct result but a window of 0.25 did.



Auto Views

Scans Search List DB View

sucrose

Find Clear

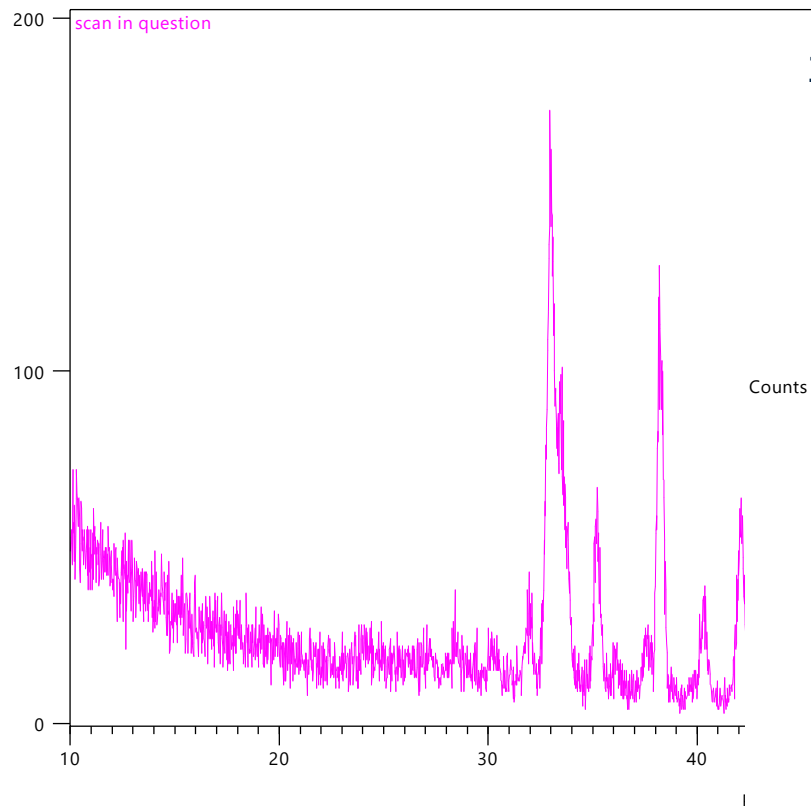
		FOM	M...	ID	Name	Formula
1	PDF 00-024-1977				(2R,3R,4S,5S,6R)-2-((2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl)oxy-6-(hydroxymethyl)oxane-3,4,5-triol Sucrose	C12H22O11

Group Duplicates

PEAK SHIFTS – SOMETIMES YOU HAVE TO SQUINT, part 1

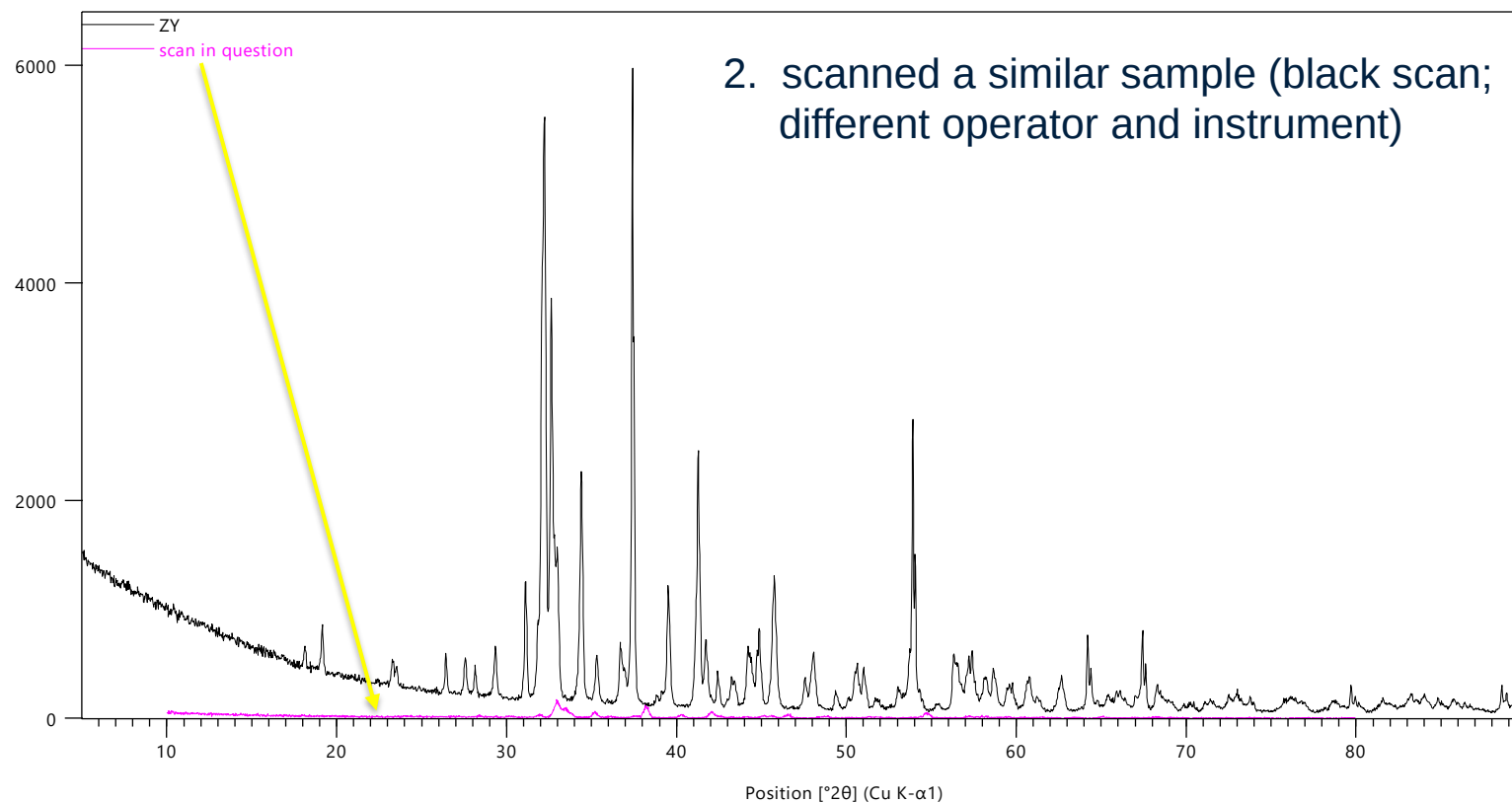


Counts



1. student run sample; had trouble identifying phase(s)

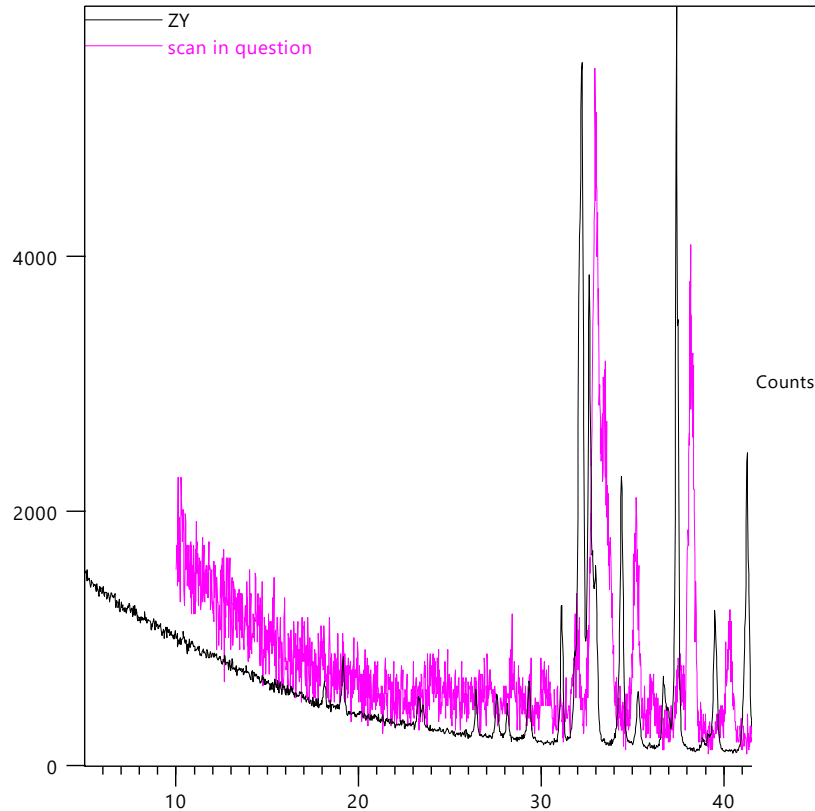
Counts



PEAK SHIFTS – SOMETIMES YOU HAVE TO SQUINT, part 2

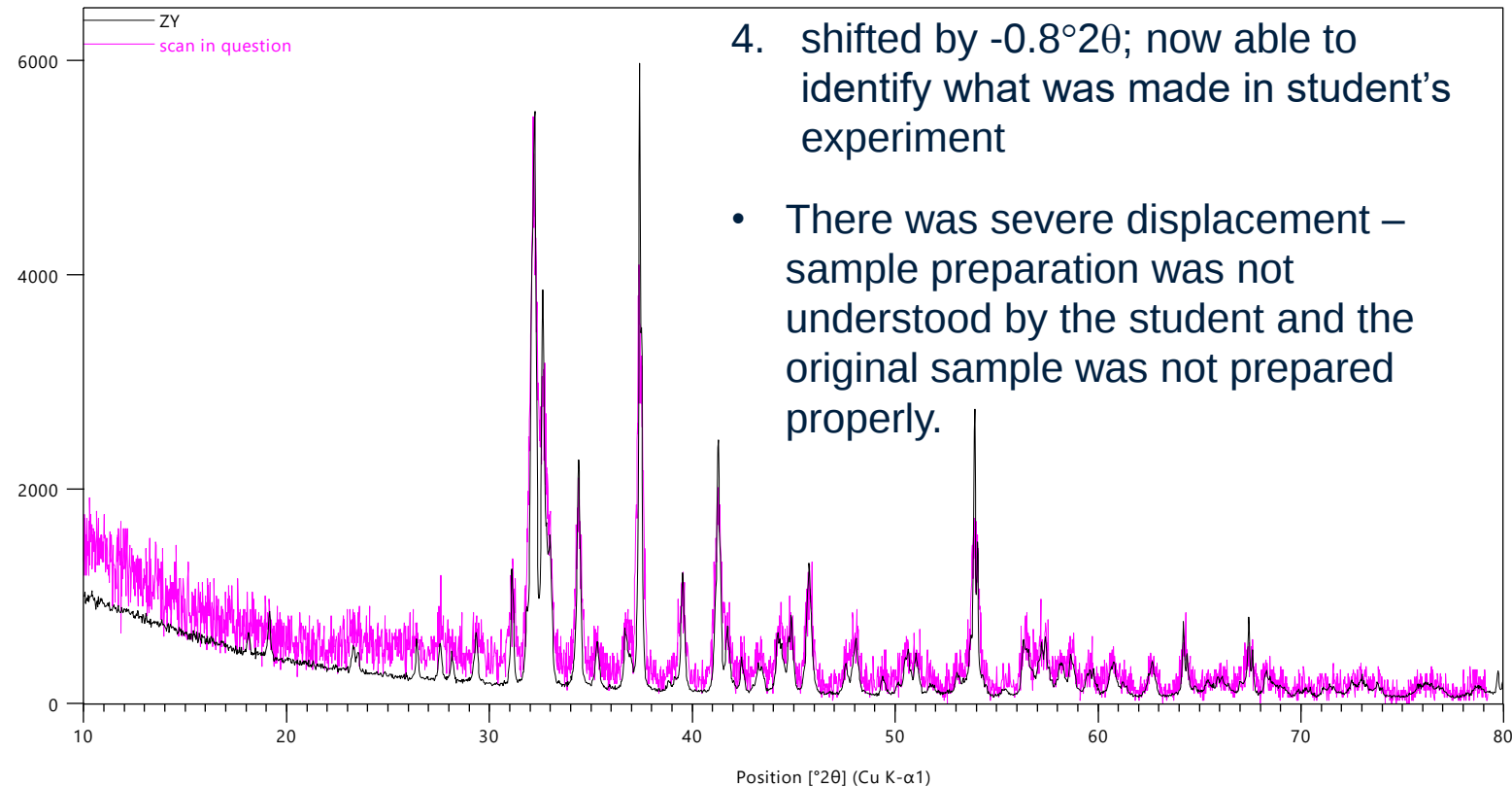


Counts



3. scaled up; if you squint you can sort of see similarities

Counts



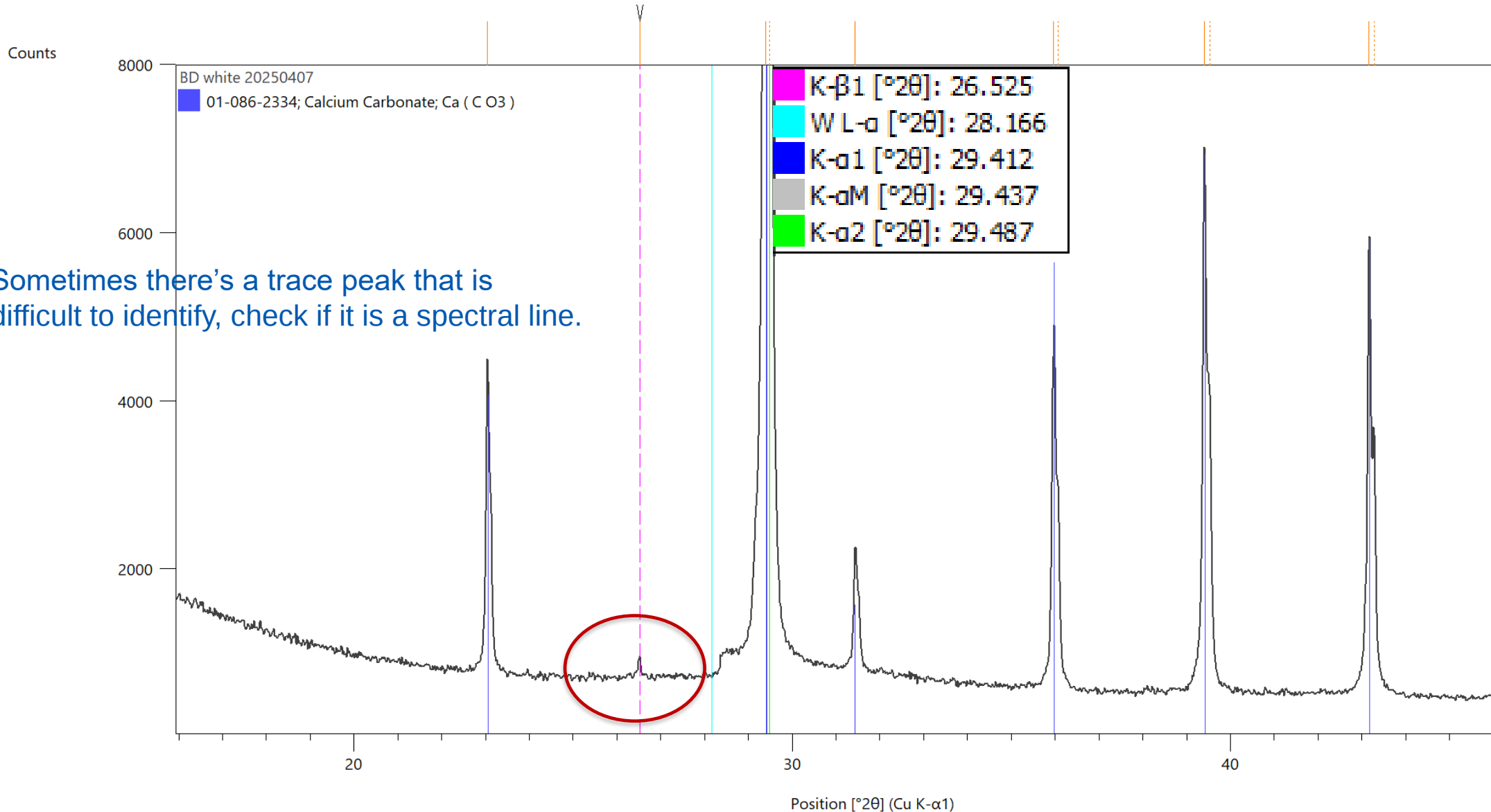
4. shifted by $-0.8^\circ 2\theta$; now able to identify what was made in student's experiment

- There was severe displacement – sample preparation was not understood by the student and the original sample was not prepared properly.

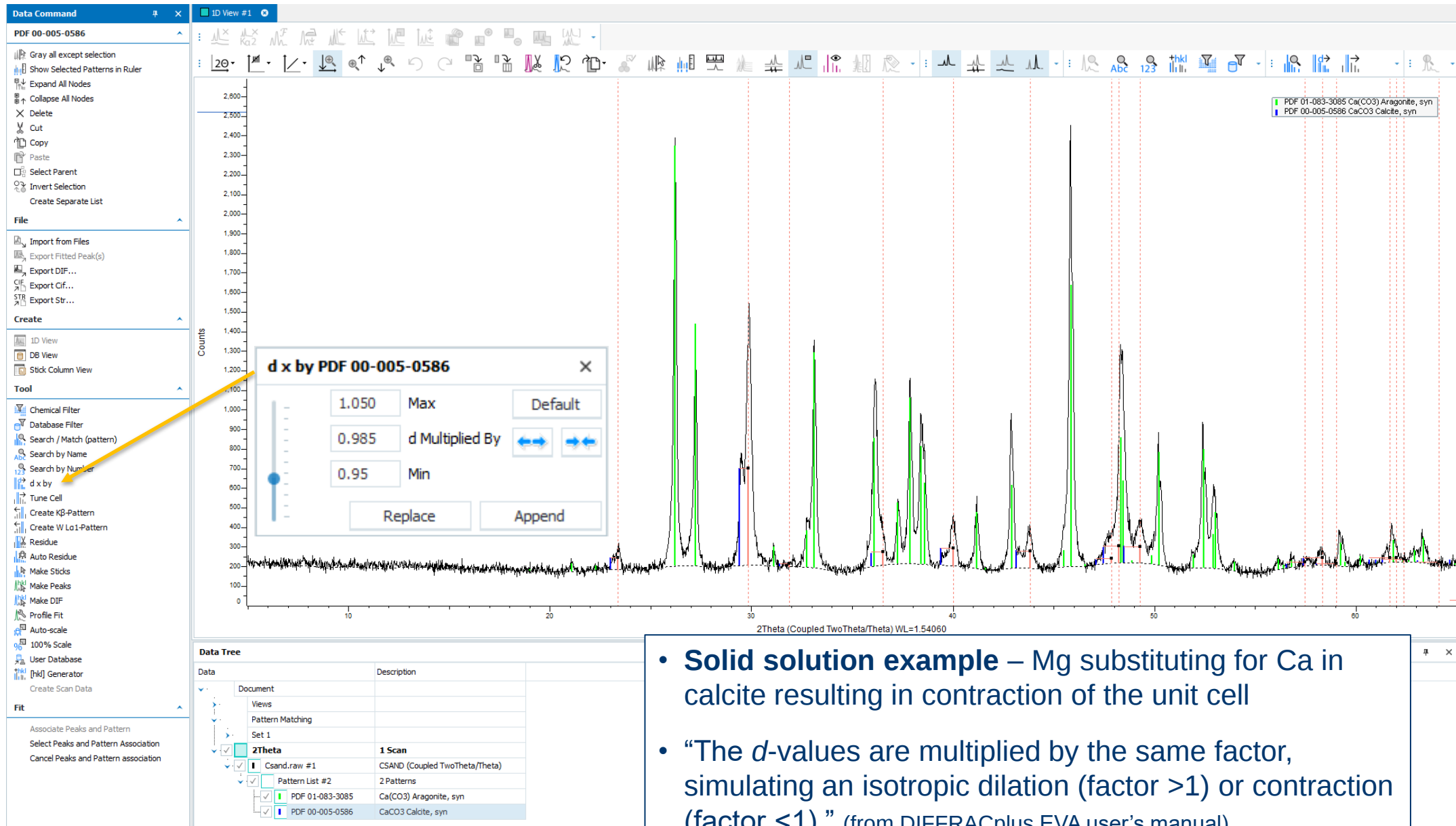
MINOR PEAKS – Check for $K\beta$ or $WL\alpha_1$ lines



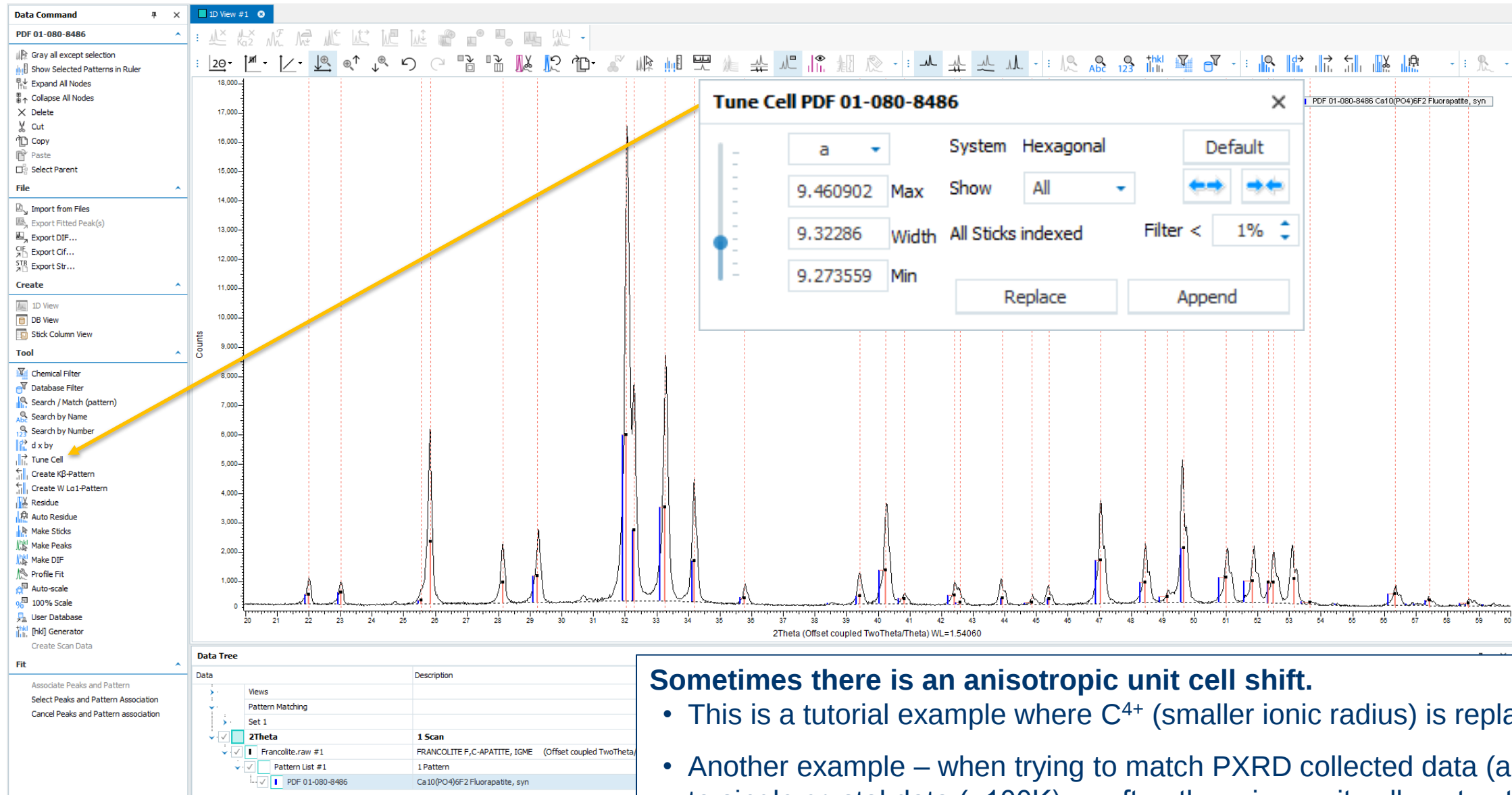
- Sometimes there's a trace peak that is difficult to identify, check if it is a spectral line.



SOLID SOLUTION – d x by (d multiplied by)



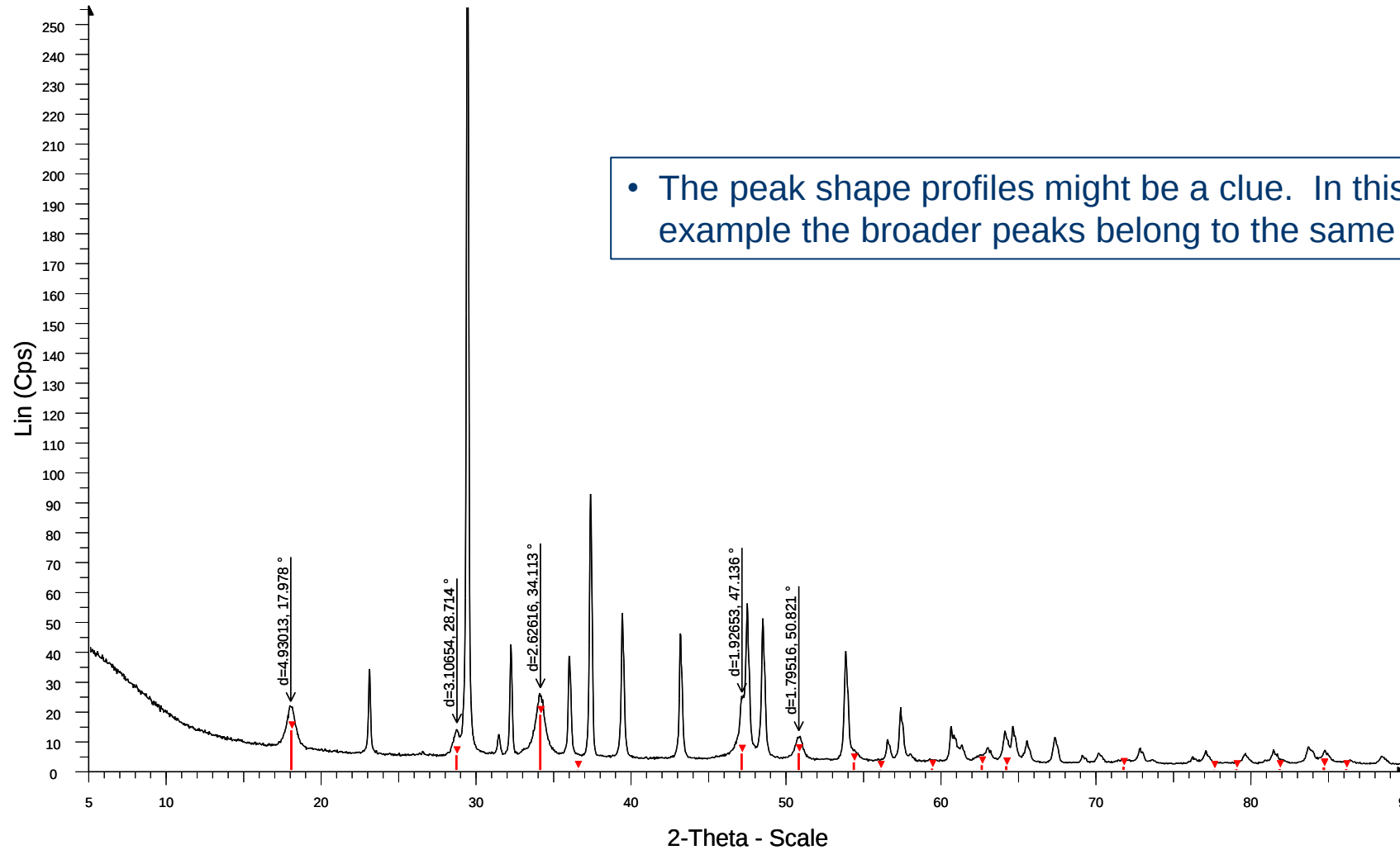
TUNE CELL – check for anisotropic unit cell shift



Sometimes there is an anisotropic unit cell shift.

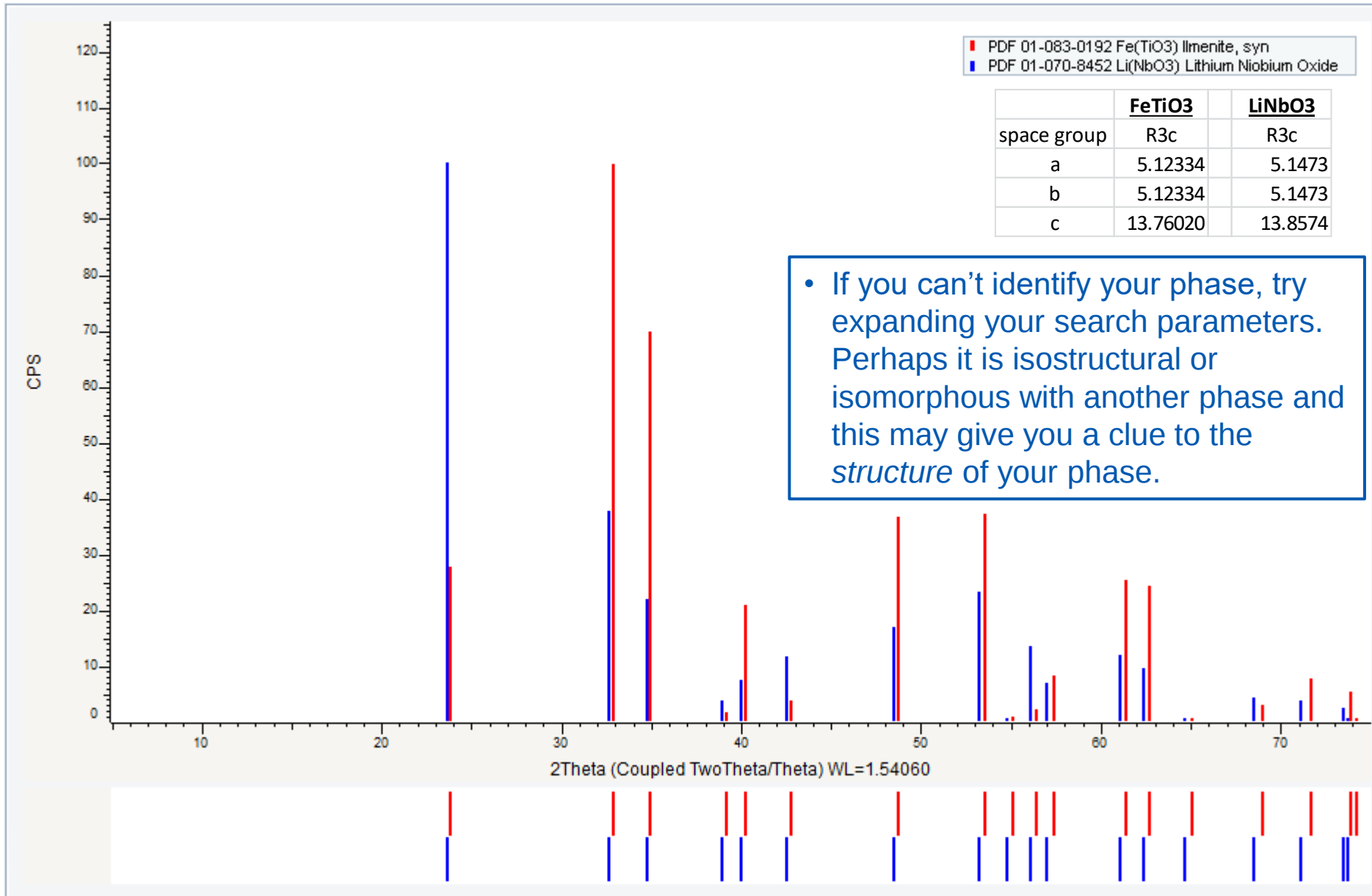
- This is a tutorial example where C^{4+} (smaller ionic radius) is replacing P^{5+}
- Another example – when trying to match PXRD collected data (ambient T) to single crystal data (~100K) ← often there is a unit cell contraction

SIMILAR PEAK SHAPES

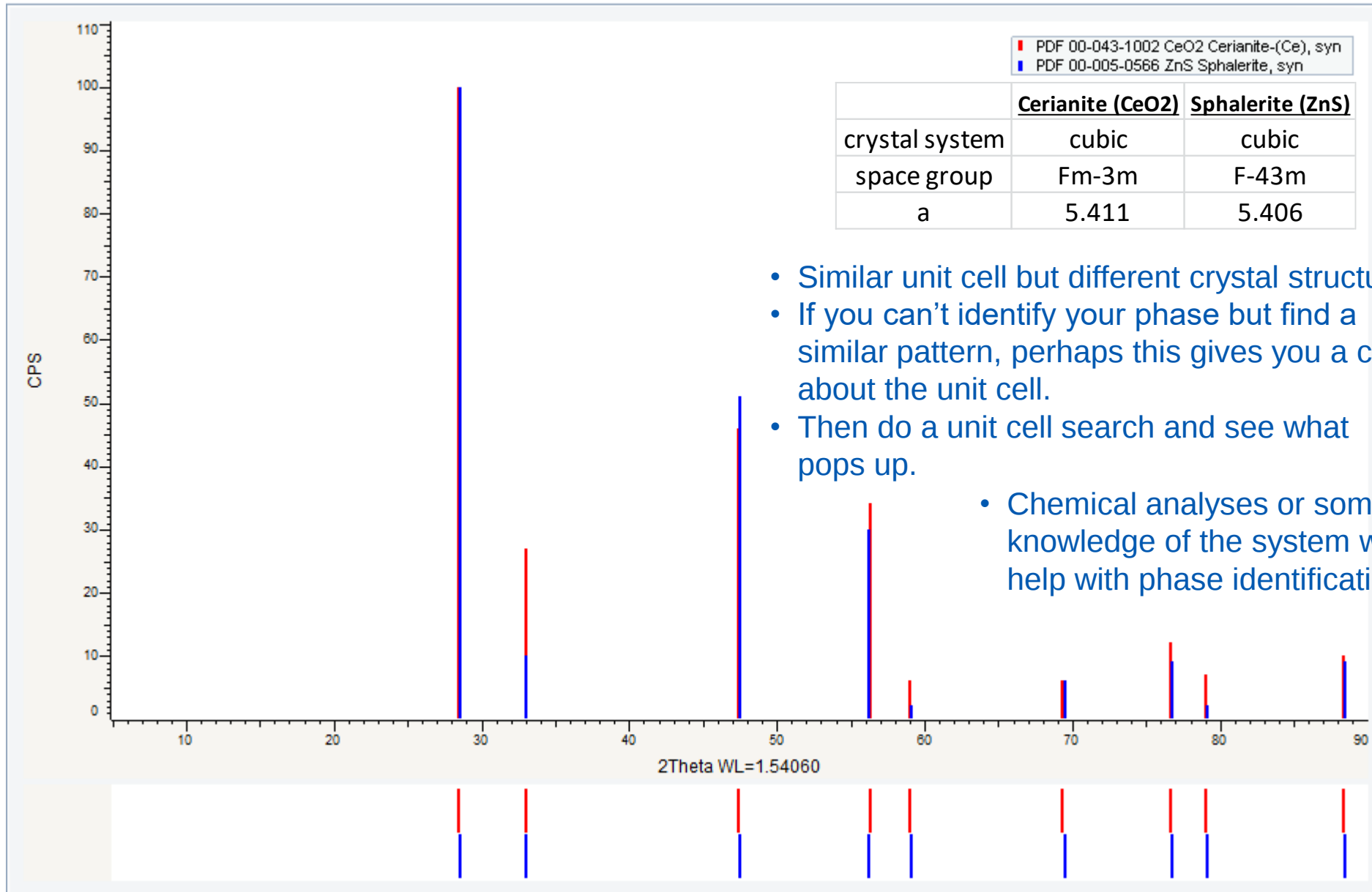


- The peak shape profiles might be a clue. In this example the broader peaks belong to the same phase.

ISOSTRUCTURAL



SIMILAR PATTERN (but not isostructural)



PHYSICAL PROPERTIES

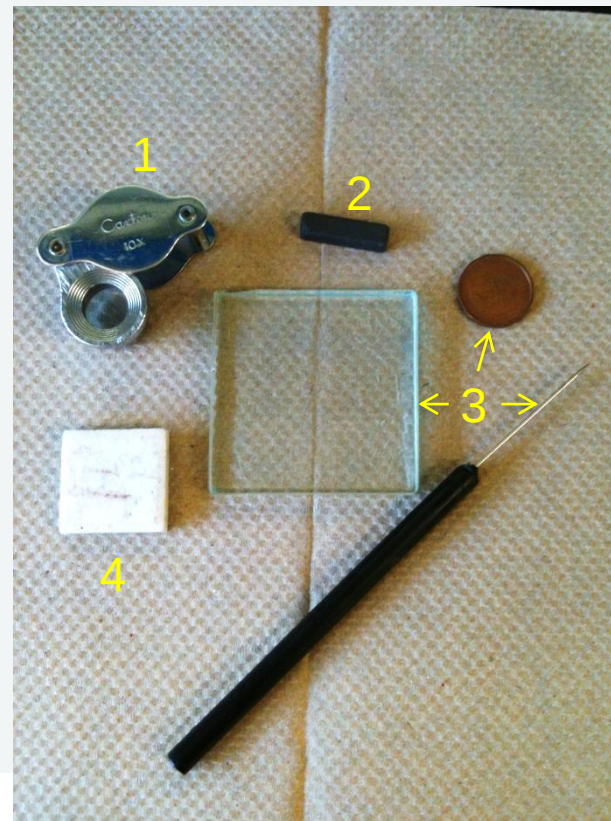


- Physical properties can be useful to help with identification

- Geologists use a basic mineral ID kit in the field

1. Visual properties – hand lens
2. Magnetism – easily tested
3. Hardness – Moh's scale
 - steel > glass > copper
4. Streak
5. Carbonate – dilute acid (not shown)

- Example



MINDSET – TIPS



Don't miss the forest for the trees

- Don't focus on specific elements too quickly
- I've had more than one student who has wasted hours trying to identify a phase when it was something simple like NaCl

Be open to possibilities

- Perhaps it is a contaminant from sample preparation or an unclean reaction vessel
- If it's a minor phase – is there a way to concentrate it or use selective dissolution?
- Maybe it's something new or not found in the database

Ask for help

- Staff at X-ray diffraction facilities
- Researchers working on the same or similar system
- Someone with fresh eyes

SUMMARY



- Phase identification is like matching fingerprints – comparing your scan to a database of known phases
- The search/match process is an interactive process between the user and software + database
- XRD is sensitive to the crystalline structure of the material; the chemistry of your phase should be confirmed by other means
 - chemical analyses and sample information help with phase identification
- User knowledge and experience is valuable to the process

THANK YOU

- UBC Chemistry Department
- Dr. Brian Patrick and Fahd Murad
- Dr. Beatriz Diaz Moreno
- And to you the audience 😊





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