X-ray Diffraction Methods Subcommittee Meeting Minutes
Wednesday, 13 March 2019
10-11:00 a.m.
Chris Gilmore, Chairman

1. Call to Order — C. Gilmore

2. Appointment of Minutes Secretary — Nicole Ernst Boris

3. Approval of Minutes from 2018
   So moved by Scott Misture.
   Seconded by John Faber.

4. Review of Mission Statement
   The X-ray Methods Subcommittee will recommend data for inclusion in the PDF by considering instrument configurations, data collection, and powder pattern calculations, emphasis on state-of-the-art methods.

5. Directors' Liaison Report — T. Ida

   Last years' motion:

   The XRD Subcommittee recommends to the Technical Committee that Headquarters explore possibilities given by traditional and advanced machine learning (e.g. partial least squares) for expanding the capabilities of the database software towards quantification.
   BoD response – positive, noting ICDD chairman at IUCr and DXC presentation/paper on this topic and more discussion at the Fall Strategy Review.

6. Short presentations

   - How to win the Reynold's Cup — S. Hillier
     Named for Bob Reynolds – Competition to promote quantitative mineral analysis– 3 samples are provided and has international participation. Suggestions on how to win: get phase ID right; factors of quantitative analysis (avoid texture); cross check results (see slides).
   - Clustering and the ICDD Databases — J. Kaduk
     As applied to Zeolite task group. Polysnap. Similarity index. MMBS.
     Jim presented zeolite clustering examples from the PDF-4+ 2019 database and named Cluster K5 and K (see slides).
   - Partial Least Squares Revisited — C. Gilmore
     Looking at PLS as a Machine Learning Method – Start with Training data (known composition) that include mixtures - important to get number of factors correct for good results – Then move to Validation data (PXRD patterns + known compositions) as independent check of training data– then finally, unknown PXRD patterns – example highlighted: AliteM1 (see slides).

7. Discussion

   The discussion portion mainly focused on the Partial Least Squares presentation.

   Chris inquired if PLS could be used for mixtures. Tom indicated, if components are known. Chris then expressed interest in working with ICDD using PLS for the database – is there a way for headquarters to process data for a project? Jim mentioned polysnap "broke" JADE™, citing fuzzy clustering. Chris then mentioned PLS might be useful for secondary analysis. He then commented that we should pursue machine learning and data mining. Jim agreed, commenting, we pitch ourselves as a smart database. Matteo commented, perhaps PLS could be used with associated minerals and the like. Tom commented, Metals and Alloys are utilizing the concept, but nothing else yet. Direction is needed from membership to move forward. This then led to a motion (below).

   Motion: The X-ray Methods Subcommittee recommends to the Technical Committee that clustering techniques be incorporated into the database as a matter of priority. A task group should be set up.

   Moved: Matteo Leoni; seconded by Jim Kaduk, 9 Yes, 0 No, 3 Abstentions - Motion passed.

8. Adjournment

How to win the Reynolds Cup!

Steve Hillier
ICDD March 2019
stephen.hillier@hutton.ac.uk

Outline

- Background of the Reynolds Cup
- Data of the Reynolds Cup
- How to win the Reynolds Cup!

Reynolds Cup Background

- Biennial competition named after Bob Reynolds (Dartmouth), established in 2000 by Douglas McCarty and Jan Srodon of ChevronTexaco and Denny Eberl of the USGS.
- Main goal: to promote and improve quantitative mineral analysis in a sportive spirit!
- Story of success (sometimes even mentioned as world championship in quantitative mineralogy).

The James Hutton Institute

Reynolds Cup Background

The James Hutton Institute

- Utilizes three sample mixtures of pure mineral phases that represent realistic sedimentary and weathered rock compositions
- Open to anyone interested in quantitative mineralogy using <u>any</u> available technique

Sample compositions/descriptions

- Mudstone
- Sandstone
- Siltstone
- Calcareous mudstone
- Saline sedimentary rock
- Sediment from an evaporate environment
- Sample representing a hydrothermal alteration environment
- Soil formed on a parent material rich in ferromagnesian minerals and amorphous soil minerals
- Petroleum shale
- Nickel laterite
- Bauxite

Mainly meant to mimic various types of sedimentary rocks and soils

Reynolds Cup background

International distribution of entries to the 9th Reynolds Cup (2018)

United States	20	Rep. Of Korea	1
Germany	11	Brazil	1
France	6	Canada	1
Australia	5	Denmark	1
United Kingdom	5	Chile	1
Poland	5	Colombia	1
Russia	5	Israel	1
Spain	4	Slovakia	1
China	3	Venezuela	1
Norway	3	Greece	1
India	2	Slovenia	1
Belgium	2	Hungary	1
Turkey	2	Italy	1
Switzerland	1	"Europe"	1

- 88 registrations
- 28 countries
- 73 finally submitted their best result

(Slide Courtesy Rieko Adriaens, organiser 9th RC)

Reynolds Cup Background

The James Hutton Institute

- How is the Reynolds Cup judged?
- 3 samples - sum total bias of all 3

$$Bias = \sum abs\left(W_{actual} - W_{submitted}\right)$$

- Where W = weight % of a given mineral
- Misidentified minerals are also counted towards bias

Reynolds Cup Background

- Top three with the lowest total bias are named and awarded with plaques and the winner receives the perpetual Reynolds Cup trophy. Other participants kept confidential.
- Winner is invited to prepare samples for the next contest

Reynolds Cup Background

- Purification
  - Hand picking
  - Sieving
  - Magnetic separation
  - Chemical treatments
  - Size fractionation (<2µm, <0.5µm, <0.2µm)
  - Synthesis
- Preparation
  - Grinding
  - Sieving (200-400µm)
  - Check for purity (XRD, XRF)
- Equilibrate
- Weighing
- Mixing
  - Ball mill
  - End over end shaking
- Homogeneity checks
  - XRD
  - XRF
- Splitting
  - Random sampling
  - Rotary splitter
- Packaging and postage

It’s a lot of work to run a Reynolds Cup!

Reynolds Cup background

Example of bias calculation

	TRUE	FOUND	Absolute error	Relative error
Quartz	20	30	10	50
K-spar	5	2	3	60
Plagioclase	7	2	5	71
Calcite	10	16	6	60
Dolomite	5	2	3	60
Pyrite	3	1	2	67
Illite/Smectite	30	34	4	13
Illite	10	5	5	50
Kaolinite	5	0	5	100
Chlorite	5	8	3	60
Total sample bias			46	

Example of the bias calculation for a simple sample (RC samples more complex)

Data of the Reynolds Cup

The 'non-clay' minerals that have been in the mixtures

- Quartz (18)
- K-feldspar (13)
- Plagioclase (14)
- Calcite (12)
- Dolomite (10)
- Magnesite (4)
- Aragonite (3)
- Huntite (1)
- Halite (6)
- Pyrite (7)
- Siderite (8)
- Barite (5)

- Gypsum (2)
- Anhydrite (2)
- Alunite (1)
- Hematite (6)
- Goethite (5)
- Magnetite (4)
- Anatase (9)
- Rutile (3)
- Ilmenite (3)
- Gibbsite (3)
- Boehmite (1)
- Fluorite (2)

- Apatite (1)
- Tourmaline (2)
- Zircon (2)
- Spinel (1)
- Opal-CT (1)
- Amphibole (3)
- Zeolite (1)
- Epidote (1)
- Birnessite (1)
- Arcanite (1)
- Amorphous (6)

As of 2012, needs updated with last 3 RC's

Data of the Reynolds Cup

Clay minerals and phyllosilicates in the mixtures

- 2:1 Dioctahedral Clays (18)
  - Smectite (montmorillonite, nontronite)
  - Mixed layered (illite-smectite, glauconite-smectite)
  - Mica/Illite (muscovite $2M_1$, illite $1M_d$, 1M)
- 2:1 Trioctahedral Clays (6)
  - Smectite (saponite)
  - Vermiculite
  - Mixed layered (corrensite)
  - Mica (biotite)
- Kaolin (15)
  - Kaolinite (well and poorly ordered)
  - Halloysite
  - Dickite
- Chlorite (11 - clinochlore, ripidolite)
- Serpentine (2 - lizardite)
- Talc (3)
- Sepiolite (1)
- Palygorskite (1)

As of 2012, needs updated with last 3 RC's

Data of the Reynolds Cup

Number of minerals in each sample

Reynolds Cup	Year	Mix1	Mix2	Mix3
RC1	2002	13	13	13
RC2	2004	13	14	12
RC3	2006	17	17	10
RC4	2008	12	13	10
RC5	2010	14	13	14
RC6	2012	14	13	14
RC7	2014	21	16	19
RC8	2016	14	12	13
RC9	2018	16	16	17

Average about 14 different minerals

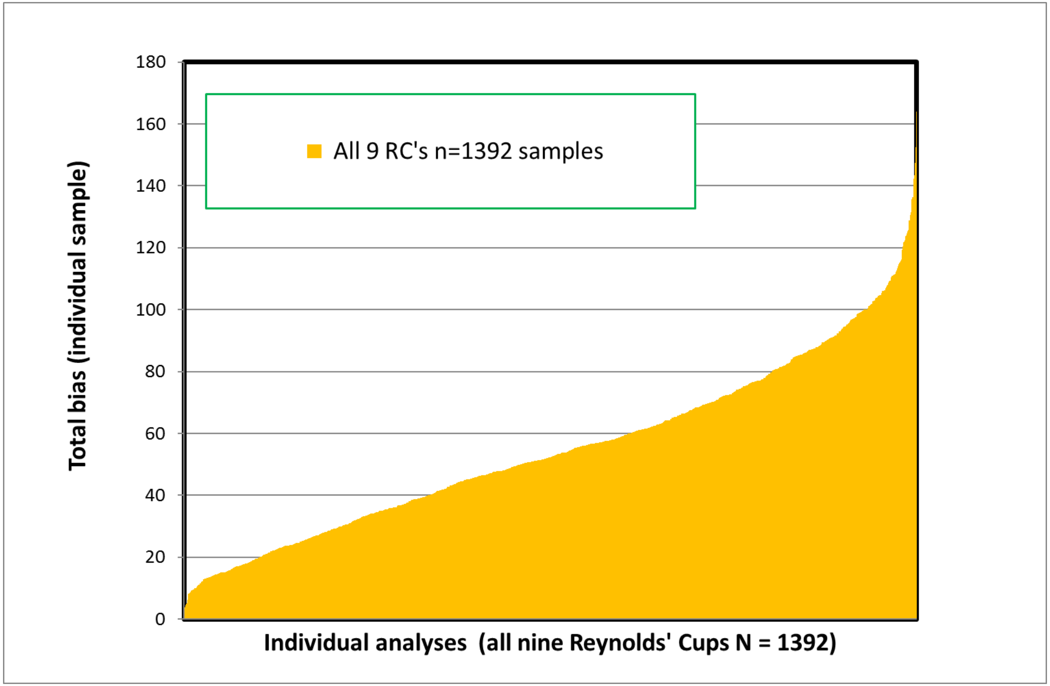
Data of the Reynolds Cup

Number of analyses returned in the last 9 Reynolds Cups

Reynolds Cup	Year	Sent out	Returned
RC1	2002	40	15
RC2	2004	60	35
RC3	2006	60	37
RC4	2008	53	43
RC5	2010	76	63
RC6	2012	74	62
RC7	2014	81	67
RC8	2016	83	69
RC9	2018	88	73
			464

Data of the Reynolds Cup

Individual RC samples



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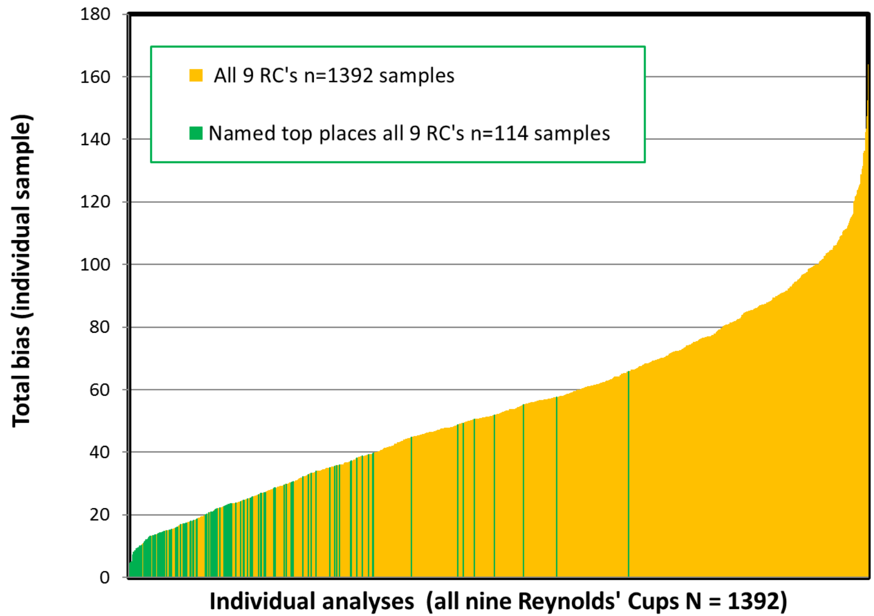
Data of the Reynolds Cup

Named top finishers (N=38 RC entries)

		1	2	3	4	5	6	7
RC1	2002	Kleeberg	Dorhmann	Eberl	Hillier			
RC2	2004	Omotoso	McCarty	Ploetz	Hillier			
RC3	2006	McCarty	Hillier	Kleeberg				
RC4	2008	Hillier	Omotoso	Kleeberg	Emmerich	Chipera	Eberl	Raven
RC5	2010	Raven	Eberl	Kleeberg	Zeelmakers	Dorhmann		
RC6	2012	Ploetz	Hillier	Kleeberg	Youjin	Dorhmann	Adriens	
RC7	2014	Kleeberg	Hillier	Dorhmann	Dietel	Emmerch	Adriens	
RC8	2016	Adriens	Raven	Hillier	Grafhoff	Dorhmann		
RC9	2018	Hillier	Lanson	Ploetz	Srodon	Raven		

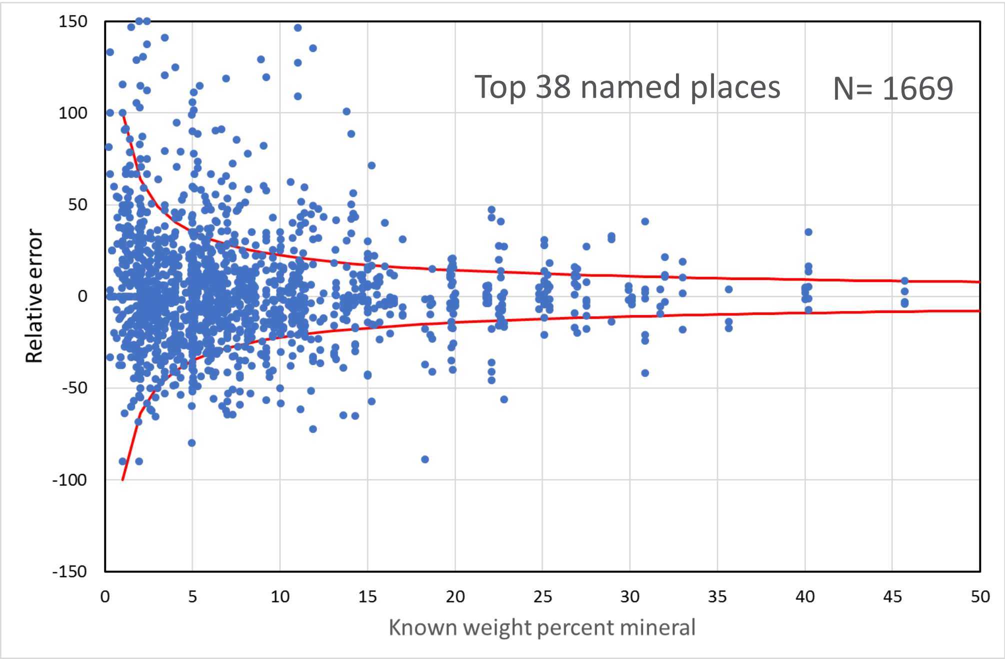
http://www.clays.org/reynolds.html

Data of the Reynolds Cup



Named top places 38 entries over the course of the 9 RC's (not all RC's are equal!)

Data of the Reynolds Cup



Uncertainty at 95% confidence

$= \pm 100X^{-0.65}$
(relative error)

$= X^{0.35}$
(absolute error)

X = wt.%

(Hillier 2003)

Data of the Reynolds Cup

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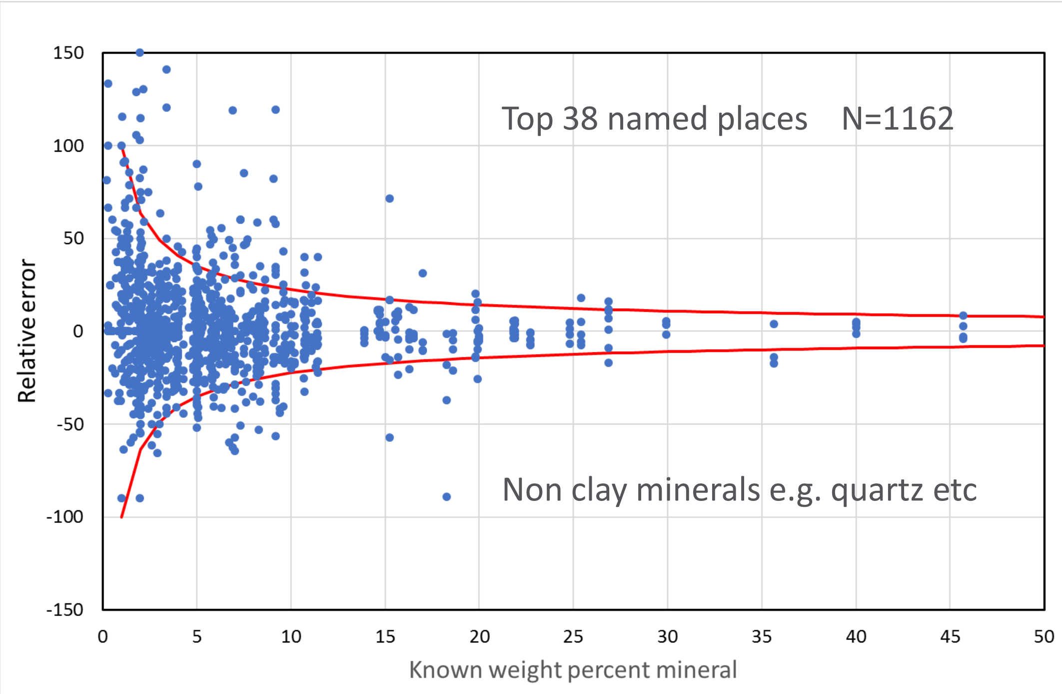

Uncertainty at 95% confidence

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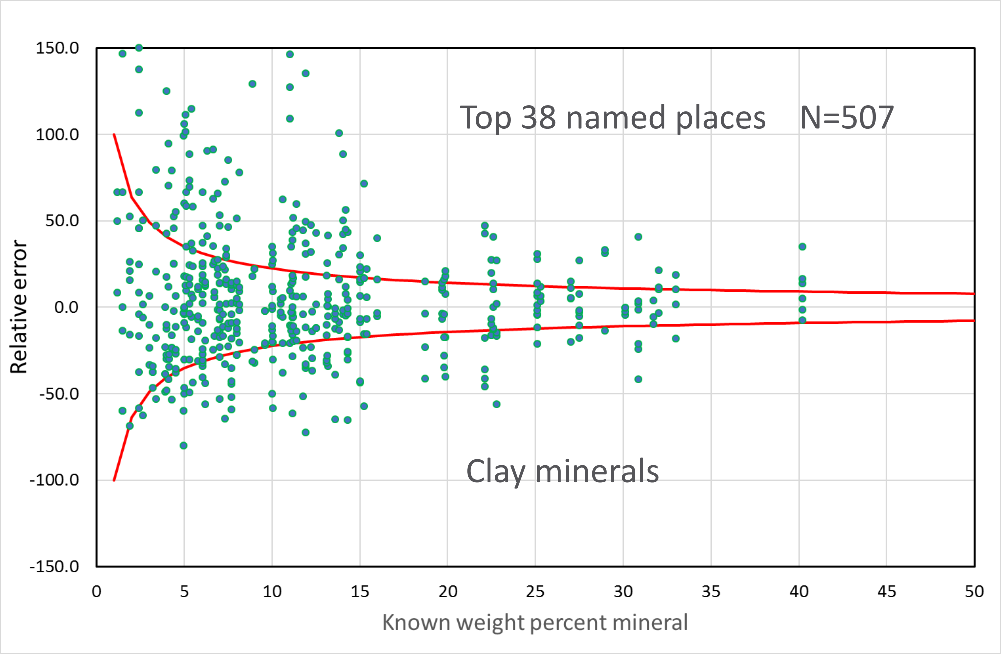
(Hillier 2003)

Data of the Reynolds



Uncertainty at 95% confidence

$= \pm 100X^{-0.65}$
(relative error)

$= X^{0.35}$
(absolute error)

X = wt.%

(Hillier 2003)

How to win the Reynolds Cup

Key recommendations on Clay Minerals Society website

http://www.clays.org/reynolds.html

- Get the identification (ID) right
  - Misidentification is the biggest source of bias
  - Clay mineral ID aided by classic oriented and treated preparations
- For quantitative analysis lots of factors but..
  - Ensure adequate particle size reduction (micronise)
  - Try to avoid texture in the specimen
  - Use full pattern methods rather than single peak
- Cross check results
  - E.g. chemical analysis – mineralogical phase analysis must be compatible with chemical analysis

How to win the Reynolds Cup

Identification is a key step - Misidentified phases

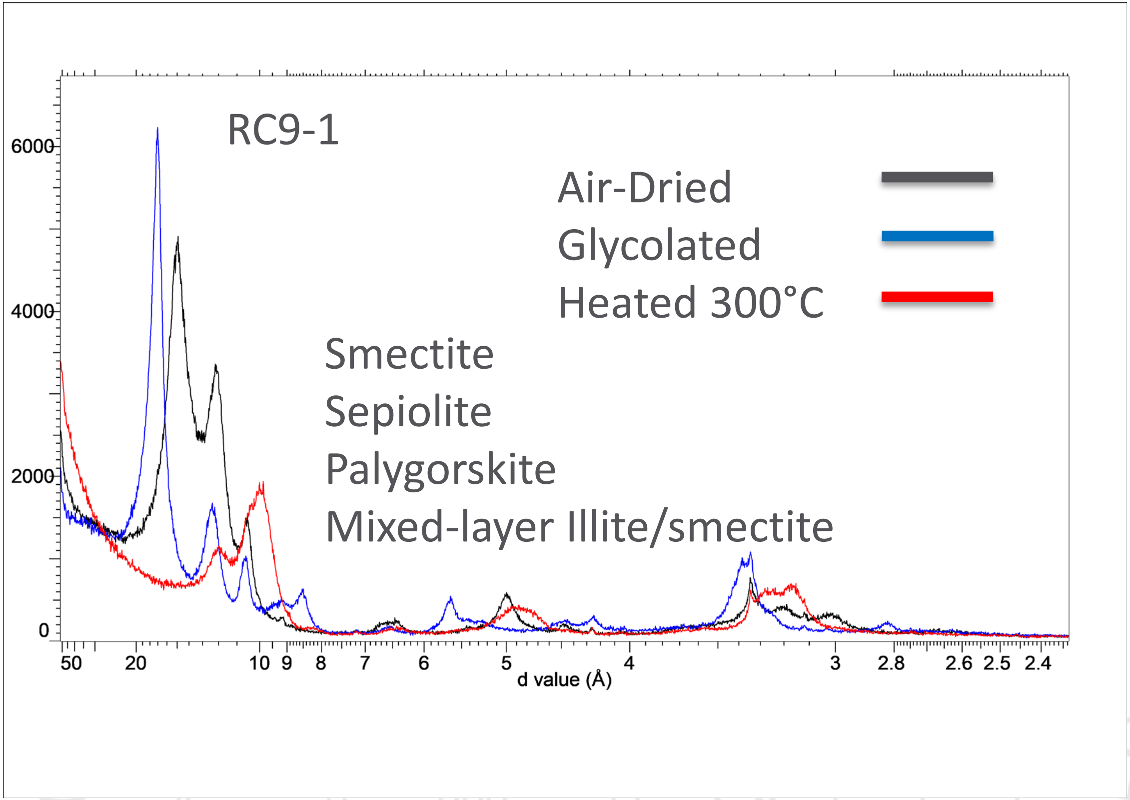
- Actinolite
- Aegerine
- Aerinite
- Akaganeite
- Albite/anorthite
- Allophane
- Alluaudite
- Almandine
- Al-Mg
- AlO
- Alumina gamma
- Aluminite
- Alunite
- Alunogen
- Amorphous
- Amorphous (Allophane)
- Amorphous KAlSi3O8
- Amorphous Si
- Amorphous SiO2
- Amorphous Volcanic Glass
- Amphibole
- Analcime
- Anatase
- Andesine
- Anhydrite
- Ankerite
- Anorthite
- Antigorite
- Antlerite
- Apatite
- Aragonite
- Arcanite
- Arsenolite As2O3
- Augite
- Barite
- Bazalt
- Berthierine
- Biotite
- Birnessite
- Bromcarnallite
- Brookite
- Brucite
- Brushite
- Bytownite
- C6H5O3PZn
- Calcite
- CaMg2Al16O27
- Carbonate-fluorapatite
- Carnallite
- CaSiO3
- Celestine
- Chabazite
- Chalcosite
- Chlorargyrite
- Chlorite Dioctahedral
- Chlorite Trioctahedral
- Chlorite-Montmorillonite(Tri)
- Chlorite-Smectite Trioctahedral
- Chlorite-vermiculite
- Chromite
- Chrysotile
- Clinochlore
- Clinoenstate
- Clinoptilolite
- ClinoPyroxene
- Clinozoisite
- Cordierite
- Corrensite
- Corundum
- Cotunnite
- Cristobalite
- Cryptohalite
- Crysotile
- Diaspore
- Dickite
- Dickite/Nacrite
- Diopside
- Dolomite
- Dolomite/Ankerite
- Elpidite
- Enstatite
- Epidote
- Euclase
- Faujasite
- Fe oxide
- Fedorite
- Feldspar (Kspar)
- Ferrihydrite
- Ferrite magnesian
- Fluorapatite
- Forsterite
- Galeite
- Garnet
- Gehlenite
- Gibbsite
- Gismondine
- Glass/Obsidian
- Glauberite
- Glauconite
- Goethite
- Gypsum
- Halite
- Halite potassian
- Halloysite
- Hectonite
- Hedenbergite
- Hematite
- Hercynite
- Heulandite
- Hexahydrite
- Hornblende
- Hotsonite
- Hyalophane
- hydrated Ca-Mg carbonate
- Hydrocalumite
- Hydrotalcite
- Hydroxyapophyllite
- Hydroxylapatite
- Hypersthene
- Illite Tri
- Ilmenite
- ilterstratified (tri)
- Iron
- Iron Silicon
- Jarosite
- KAlSiO4
- Kaolinite
- kaolinite/smectite
- Kaolinite-Chlorite
- K-feldspar
- Kieserite
- K-rich Chlorite
- Kutnohorite
- Laueite
- Laumonite
- Lepidocrocite
- Leucite
- Lime
- Lithosite
- Lizardite
- Magnesioferrite
- Magnesite
- Magnetite
- Malachite
- Manganite
- Melantenite
- Mg7Zn3
- Mg-calcite
- MgSO4
- Mica
- Mica Trioctahedral
- Mica-Vermiculite Trioctahedral
- Microcline
- Missing
- Monazite
- Monohydrocalcite
- Montmorillonite (Tri)
- Moschellandsbergite
- Mullite
- Nacrite
- Na-Feldspar
- Natrolite
- Nepheline
- Nitride Silicon
- Nordstrandite
- Norrishite
- Oligoclase
- Olivine
- Opal
- Opal CT
- Orthoclase
- OrthoPyroxene
- Osumilite
- Others not precisely identified
- oxide 1
- oxide 2
- Palygorskite
- Periclase
- Perovskite
- Phillipsite
- Phlogopite (2M1)
- Phlogopite (mica-trioctahedral)
- phosphate hydrate
- Plagioclase
- Portlandite
- Potarite
- Prehnite
- Pseudobrookite
- Pumpellyite
- Pyrite
- Pyrolusite
- pyrophyllite 1T
- pyrophyllite 2M
- Pyroxene
- Pyroxene (Augite)
- Pyroxene (Ferroan Diopside)
- Pyrrhotite
- Rectorite
- Reyerite
- Rhodochrosite
- Rhodonite
- Rodolicoite
- Rutile
- Sanidine
- Saponite
- Sauconite
- Schorl
- Sepiolite
- Serpentine
- Siderite
- Siderite (Mn-rich)
- Siderite(not Mg)
- Silicon
- Silicon dioxide
- Sillimanite
- Smectite trioctahedral
- Smithsonite
- Sodalite
- Spencerite
- Sphalerite iron
- Spinel
- Staurolite
- Strontianite
- Sylvite
- Syngenite
- Szomolnokite
- Talc
- Thenardite
- Thermonatrite
- Titanite
- Titanomagnetite
- Tobermorite
- Tourmaline
- Trimerite
- Trydymite
- Tungstite
- Unidentified
- Unnamed hydrate
- Vaterite
- Vauxite
- Vermiculite
- Vermiculite Trioctahedral
- Vermiculite/illite
- Vermiculite-Smectite Trioctahedral
- Vesuvianite
- Wagnerite
- Wavellite
- Whitlockite
- Whitmoreite
- Wollastonite
- Wroewolfeite
- Wuestite
- Zeolite
- Zeophyllite
- Zinnwaldite
- Zircon
- Zirconium sulphate hydroxide hydrate
- Zoisite

260!

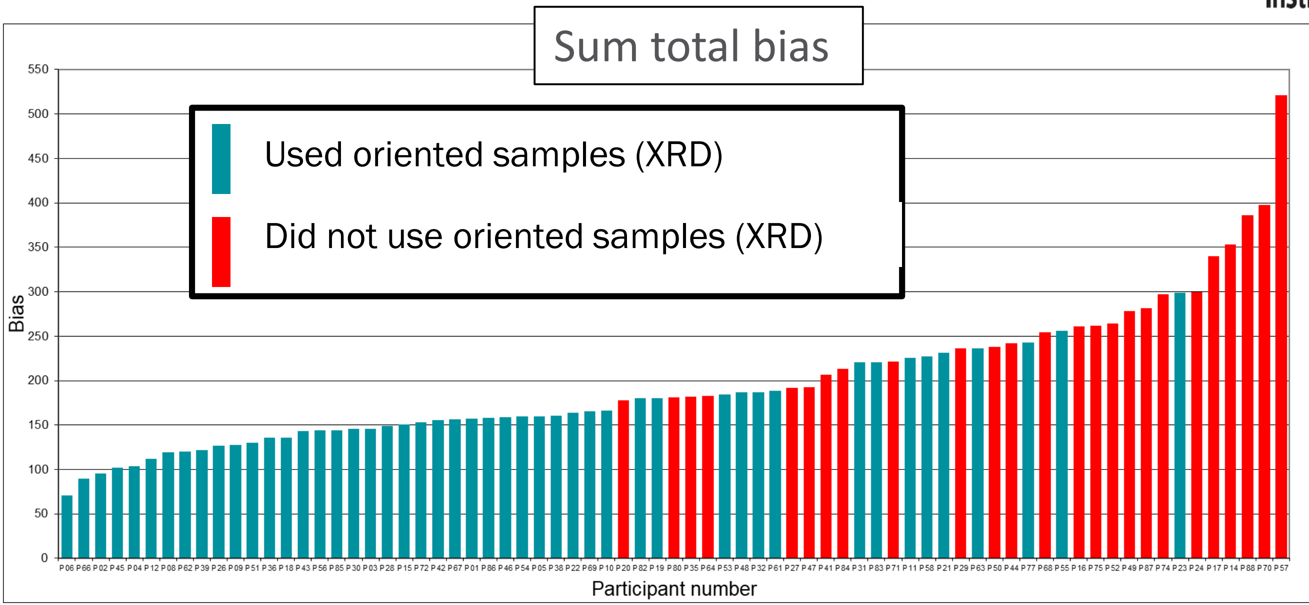
As of 2012, needs updated

How to win the Reynolds Cup

Use oriented clay preparations to help ID the clay minerals

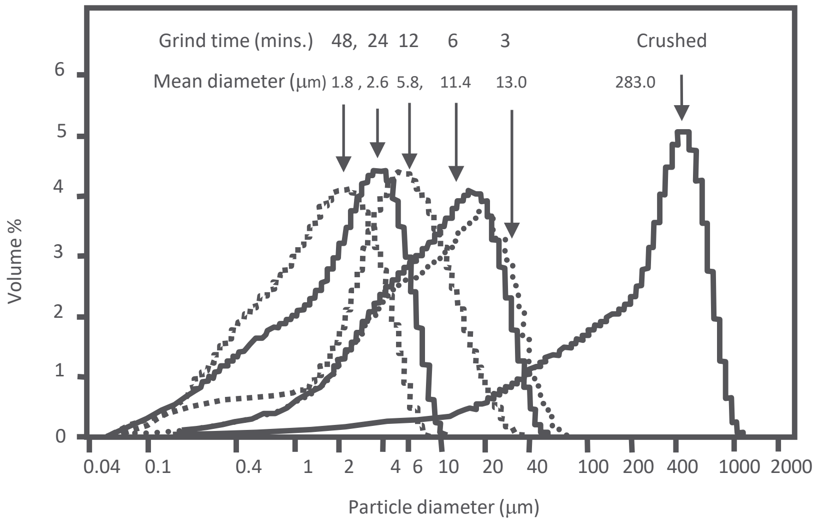


How to win the Reynolds Cup



How to win the Reynolds Cup

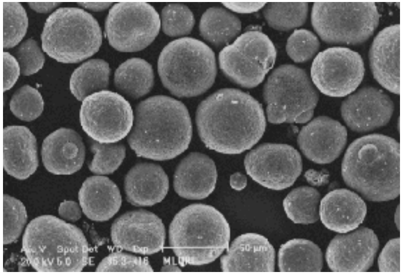
- For optimum particle size, best method micronizing with something like the McCrone Mill
  - Good at reducing (not smearing) particle size distribution



Example is for crushed quartz

How to win the Reynolds Cup

- Various method of <u>attempting</u> to make a random powder
- Top, back or side loading
  - Draw backs - reproducibility very difficult to guarantee
  - Advantages – simple
- Best method is spray drying
  - Draw backs – need a couple of grams
  - Need the equipment
  - Advantages – <u>extremely reproducible</u>
    - <u>Why? Because It is a random powder</u>



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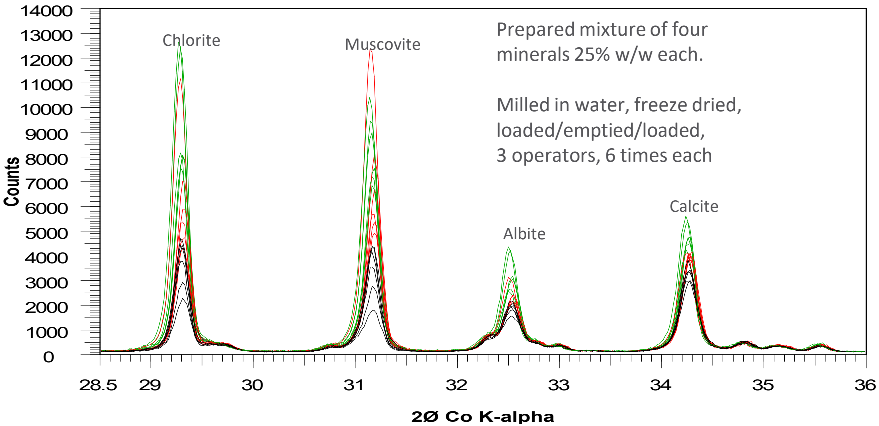
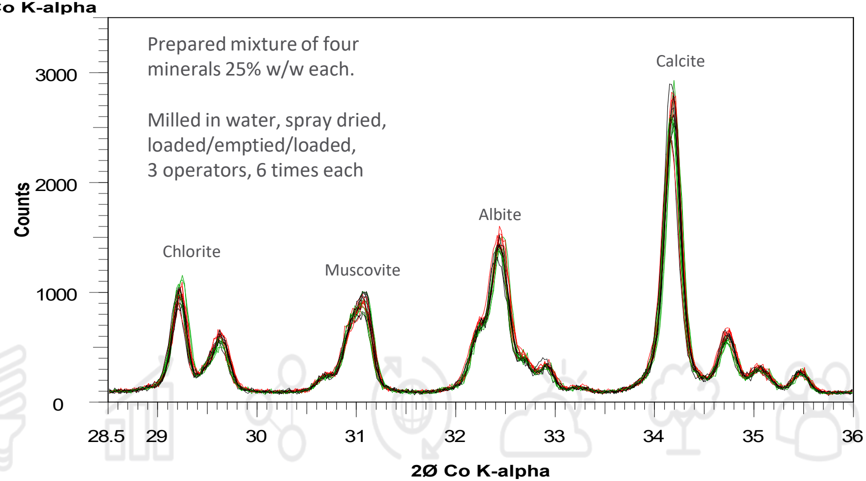
How to win the Reynolds Cup





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How to win the Reynolds Cup

Use pattern summation

Reynolds Cup	Year	% Rietveld	% Summation
RC1	2002	27	20
RC2	2004	54	20
RC3	2006	54	14
RC4	2008	63	28
RC5	2010	73	17
RC6	2012	63	23
RC7	2014	60	18
RC8	2016	74	10
RC9	2018	81	18
	Average	**65**	**18**

How to win the Reynolds Cup

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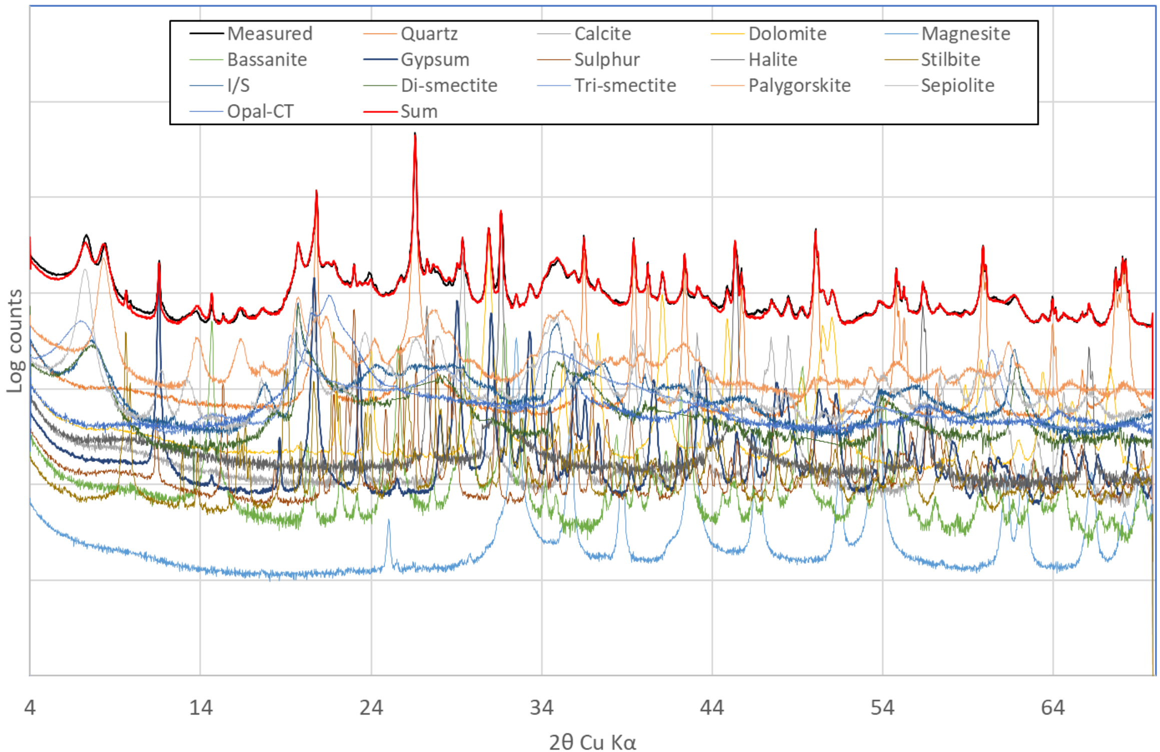
RC9-1



How to come 2nd in the Reynolds Cup (the best place to finish!)

- Automated full pattern summation
- Couples phase identification and quantification
- Testing on previous RC samples
  - RC3 = 2nd/39;
  - RC4 = 2nd/44;
  - RC5 = 2nd/64;
  - RC6 = 5th/63;
  - RC7 = 9th/68;
  - RC8 = 1st/70;
  - RC9 = 2nd/74

Next (10th) Reynolds Cup early 2020

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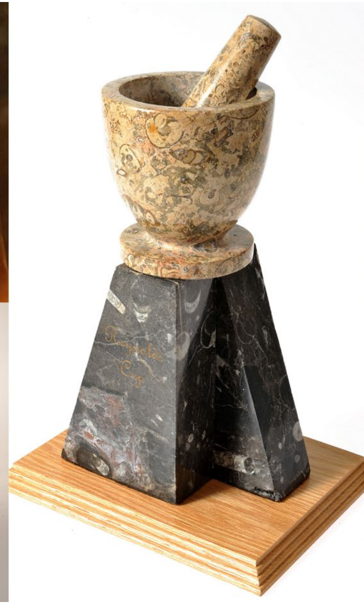
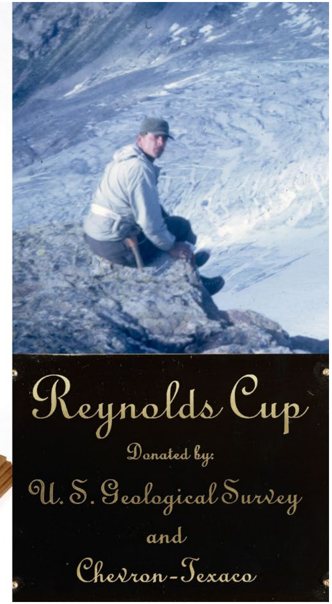




Acknowledgements - Mark Raven and Reiko Adriaens for various slides and all previous organisers and participants of the Reynolds Cup

Application of Cluster Analysis in the Zeolite Task Group

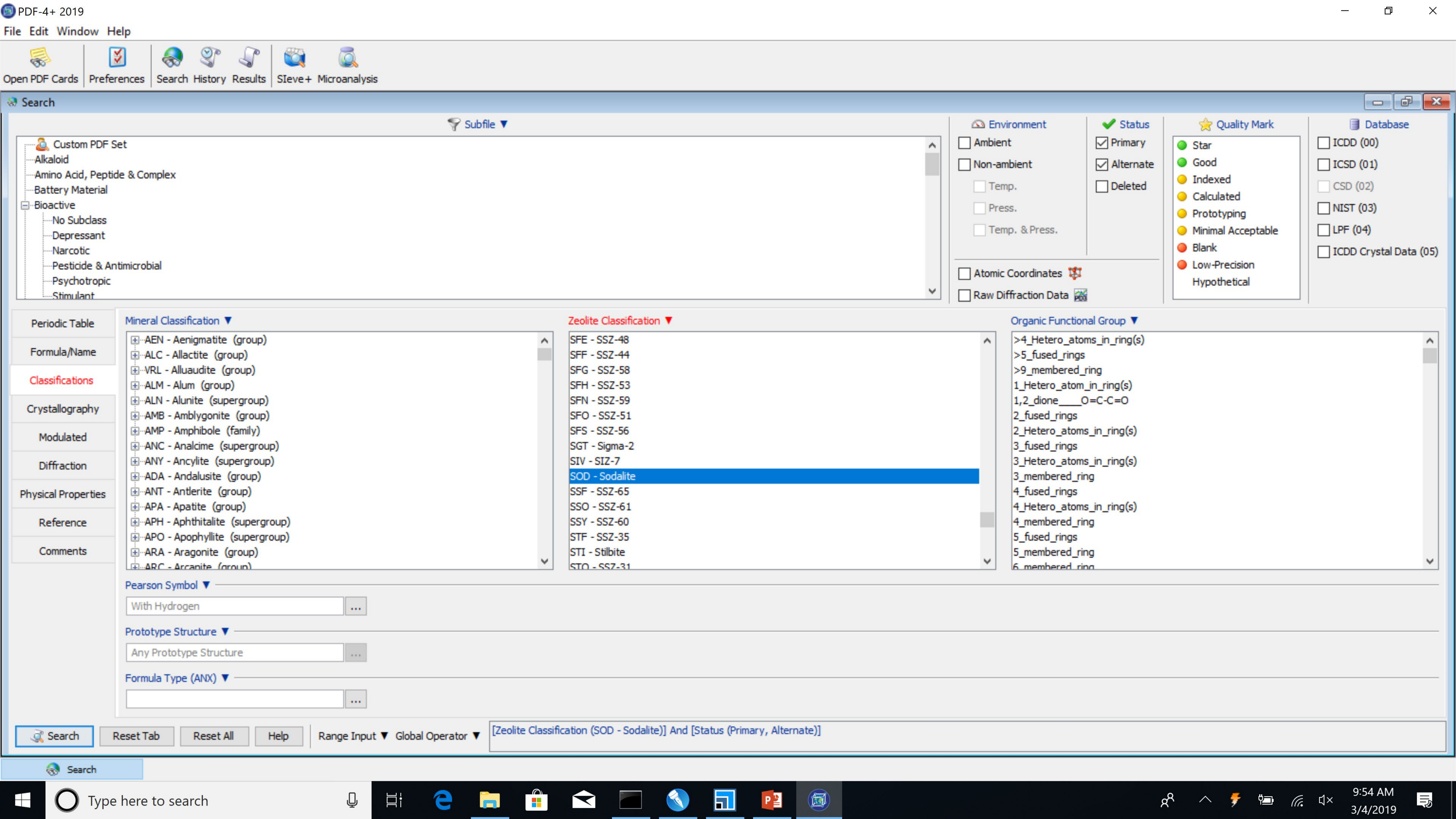
NORTH CENTRAL COLLEGE
NAPERVILLE, ILLINOIS
Founded 1861

James A. Kaduk
Illinois Institute of Technology
North Central College
Kaduk@polycrystallography.com

ILLINOIS INSTITUTE OF TECHNOLOGY

ICDD
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

greener
Non Scratch
Scouring Pads


PDF-4+ 2019
File Edit Window Help
Open PDF Cards
Preferences
Search
History
Results
SIeve+
Microanalysis
Search
Subfile
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Psychotropic
Stimulant
Environment
Ambient
Non-ambient
Temp.
Press.
Temp. & Press.
Atomic Coordinates
Raw Diffraction Data
Status
Primary
Alternate
Deleted
Quality Mark
Star
Good
Indexed
Calculated
Prototyping
Minimal Acceptable
Blank
Low-Precision
Hypothetical
Database
ICDD (00)
ICSD (01)
CSD (02)
NIST (03)
LPF (04)
ICDD Crystal Data (05)
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Mineral Classification
AEN - Aenigmatite (group)
ALC - Allactite (group)
VRL - Alluaudite (group)
ALM - Alum (group)
ALN - Alunite (supergroup)
AMB - Amblygonite (group)
AMP - Amphibole (family)
ANC - Analcime (supergroup)
ANY - Ancylite (supergroup)
ADA - Andalusite (group)
ANT - Antlerite (group)
APA - Apatite (group)
APH - Aphthitalite (supergroup)
APO - Apophyllite (supergroup)
ARA - Aragonite (group)
Zeolite Classification
SFE - SSZ-48
SFF - SSZ-44
SFG - SSZ-58
SFH - SSZ-53
SFN - SSZ-59
SFO - SSZ-51
SFS - SSZ-56
SGT - Sigma-2
SIV - SIZ-7
SOD - Sodalite
SSF - SSZ-65
SSO - SSZ-61
SSY - SSZ-60
STF - SSZ-35
STI - Stilbite
Organic Functional Group
>4_Hetero_atoms_in_ring(s)
>5_fused_rings
>9_membered_ring
1_Hetero_atom_in_ring(s)
1,2_dione____O=C-C=O
2_fused_rings
2_Hetero_atoms_in_ring(s)
3_fused_rings
3_Hetero_atoms_in_ring(s)
3_membered_ring
4_fused_rings
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5_membered_ring
Pearson Symbol
With Hydrogen
Prototype Structure
Any Prototype Structure
Formula Type (ANX)
Search
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Help
Range Input
Global Operator
[Zeolite Classification (SOD - Sodalite)] And [Status (Primary, Alternate)]
Search
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PDF #	QM	Chemical Formula	Compound Name	Mineral Name	D1 (Å)	D2 (Å)	D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1
00-002-0351	I	$Al_6 Na_8 Si_6 O_{24} Cl_2$	Aluminum Sodium Silicate Chloride	Sodalite	3.640000	2.100000	2.380000	C	P-43n	8.890	8.890	702.60	6.2
00-011-0401	I	$Na_4 Al_3 Si_3 O_{12} (OH)$	Sodium Aluminum Silicate Hydroxide		3.630000	6.280000	2.560000	C	P-43n	8.874	8.874	698.81	6.2
00-011-0491	B	$(Fe, Mn)_4 Be_3 Si_3 O_{12} S$	Iron Manganese Beryllium Sulfide Silicate	Danalite	3.350000	1.932000	1.012000	C	P-43n	8.207	8.207	552.78	4.0
00-013-0114	I	$Fe Zn_3 Be_3 Si_3 O_{12} S$	Iron Zinc Beryllium Silicate Sulfide	Genthelvite	3.330000	2.174000	1.918000	C	P-43n	8.150	8.150	541.34	4.0
00-014-0017	O	$(NH_4)_3 Al_3 Si_3 O_{12} Cl$	Ammonium Aluminum Chloride Silicate		3.644000	6.330000	2.580000	C	I	8.930	8.930	712.12	6.3
00-015-0253	I	$(Mn, Fe, Zn)_4 Be_3 Si_3 O_{12} S$	Manganese Beryllium Sulfide Silicate	Helvite	3.370000	1.947000	1.124000	C	P-43n	8.261	8.261	563.76	3.6
00-016-0612	O	$Na_2O \cdot Al_2O_3 \cdot 2.1 SiO_2 \cdot x H_2O$	Sodium Aluminum Oxide Silicate Hydrate		3.630000	2.810000	2.560000	X					6.2
00-017-0538	I	$Na_8 Al_6 Si_6 O_{24} SO_4$	Sodium Aluminum Sulfate Silicate	Nosean, syn	3.710000	2.628000	6.450000	C	P-43m	9.078	9.078	748.07	9.0
00-017-0749	S	$Na_6 Ca_2 Al_6 Si_6 O_{24} (SO_4)_2$	Sodium Calcium Aluminum Silicate Sulfate	Lazurite-C	3.710000	2.622000	2.872000	C	P-43m	9.090	9.090	751.09	6.4
00-019-1182	I	$Na_4 Al Be Si_4 O_{12} (Cl, S)$	Sodium Aluminum Beryllium Chloride Silicate	Tugtupite	3.520000	6.130000	3.570000	T	I-4	8.583	8.817	649.53	6.1
00-020-1087	I	$(Na, Ca)_8 (Si, Al)_{12} O_{24} (S...$	Sodium Calcium Aluminum Silicate Sulfate	Haüyne	3.720000	2.623000	6.470000	C	P-43n	9.082	9.082	749.11	6.4
00-021-1099	S	$Na_8 Al_6 Si_6 O_{24} SO_4$	Sodium Aluminum Silicate Sulfate	Nosean	3.710000	6.440000	2.628000	C		9.100	9.100	753.57	6.4
00-022-1809	I	$C_4 H_{12} Al N O_{12} Si_5$	Tetramethyl Ammonium Aluminum Silicate		3.670000	4.490000	6.360000	T	I-4	8.975	8.975	722.94	6.3
00-024-0893	O	$Na_4 (Al, Ga)_3 Si_3 O_{12} (OH)$	Sodium Aluminum Gallium Silicate Hydroxide		3.650000	2.830000	2.590000	C	P-43n	8.880	8.880	700.23	4.1
00-024-1045	B	$Na_8 Al_6 Si_6 O_{24} CO_3$	Sodium Aluminum Silicate Carbonate		6.260000	3.630000	2.578000	C		17.709	17.709	5553.70	10.2
00-025-0797	B	$Na_6 Ca_2 Al_3 Ga_3 Si_6 O_{24} (CrO_4)_2$	Sodium Calcium Aluminum Gallium Chromium Oxide Silicate		3.746000	3.243000	2.164000	C	P-43n	9.180	9.180	773.62	6.5
00-025-0798	I	$Na_6 Ca_2 Al_2 Ga_4 Si_6 O_{24} (MoO_4)_2$	Sodium Calcium Aluminum Gallium Molybdenum Oxide Silicate		3.763000	2.658000	2.461000	C	P-43n	9.220	9.220	783.78	6.5
00-025-0799	I	$Na_6 Ca_2 Al_2 Ga_4 Si_6 O_{24} (WO_4)_2$	Sodium Calcium Aluminum Gallium Tungsten Oxide Silicate		3.765000	2.305000	2.661000	C	P-43n	9.220	9.220	783.78	6.5
00-025-0802	I	$Na_6 Ca_2 Al_6 Si_6 O_{24} (SO_4)_2$	Sodium Calcium Aluminum Silicate Sulfate	Haüyne, syn	3.711000	6.451000	2.624000	C	P-43n	9.095	9.095	752.33	6.4
00-027-0066	I	$Ca_2 Al_2 Si O_6 (OH)_2$	Calcium Aluminum Silicate Hydroxide	Bicchulite, syn	2.793000	3.610000	2.081000	C	I-43m	8.824	8.824	687.11	4.4
00-029-1184	B	$Na_6 Ca_2 Al_6 Ge_6 O_{24} (WO_4)_2$	Sodium Calcium Aluminum Germanium Tungsten Oxide		3.810000	2.694000	2.324000	C	P-43n	9.326	9.326	811.12	6.5
00-029-1186	I	$Na_6 Ca_2 Al_6 Si_6 O_{24} (TeO_4)_2$	Sodium Calcium Aluminum Silicate Tellurate		3.720000	2.635000	4.560000	C	P-43n	9.120	9.120	758.55	6.4
00-029-1221	B	$Na_6 Pb_2 Al_6 Si_6 O_{24} (SO_4)_2$	Sodium Lead Aluminum Silicate Sulfate		3.720000	2.637000	2.148000	C	P-43n	9.117	9.117	757.80	6.4
00-031-1271	O	$1.08 Na_2O \cdot Al_2O_3 \cdot 1.68 SiO_2 \cdot 1.8...$	Sodium Aluminum Silicate Hydrate		3.670000	6.360000	2.590000	C		8.980	8.980	724.15	6.3
00-032-1031	S	$Na_4 Al_3 Si_3 O_{12} I$	Sodium Aluminum Iodide Silicate		3.680000	2.125000	2.409000	C	P-43n	9.011	9.011	731.65	6.3
00-032-1032	S	$Na_4 Al_3 Si_3 O_{12} Br$	Sodium Aluminum Bromide Silicate		3.650000	2.106000	2.388000	C	P-43n	8.933	8.933	712.84	6.3
00-033-1164	S	$Ag_4 Al_3 Si_3 O_{12} I$	Silver Aluminum Silicate Iodide		3.650000	2.105000	2.387000	C	P-43n	8.930	8.930	712.12	6.3
00-035-0002	B	$Ca_2 Si O_2 F_2$	Calcium Fluoride Silicate		3.100000	3.205000	3.615000	T		6.937	8.488	408.46	6.9
00-035-0032	O	$Na_4 Si_3 Al_3 O_{12} Br$	Sodium Aluminum Bromide Silicate		3.650000	2.450000	2.110000	C	P-43n	8.932	8.932	712.60	6.3
00-037-0196	I	$Na_8 Al_6 Si_6 O_{24} (CN)_2 \cdot x H_2O$	Sodium Aluminum Cyanide Silicate Hydrate		3.640000	6.310000	2.580000	C	I	8.921	8.921	709.97	6.3
00-037-0473	S	$Na_6 Ca_2 Al_6 Si_6 O_{24} (SO_4)_2$	Sodium Calcium Aluminum Silicate Sulfate	Haüyne	3.723000	2.633000	2.150000	C	P-43n	9.120	9.120	758.53	6.4
00-037-0476	S	$Na_4 Al_3 Si_3 O_{12} Cl$	Sodium Aluminum Silicate Chloride	Sodalite	3.624000	6.280000	2.093000	C	P-43n	8.878	8.878	699.85	6.2
00-038-0021	I	$Na_8 (Al_6 Si_6 O_{24}) (NO_2)_2 \cdot 3 H_2O$	Sodium Aluminum Nitrite Silicate Hydrate		3.660000	6.350000	2.110000	C		8.943	8.943	715.24	6.3

[Zeolite Classification (SOD - Sodalite)] And [Status (Primary, Alternate)]

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Na4 Al3 Si3 O12 Cl - 00-037-0476

Help

Unit Cell: 1 1 1

Show Atom Labels

Show Polyhedra

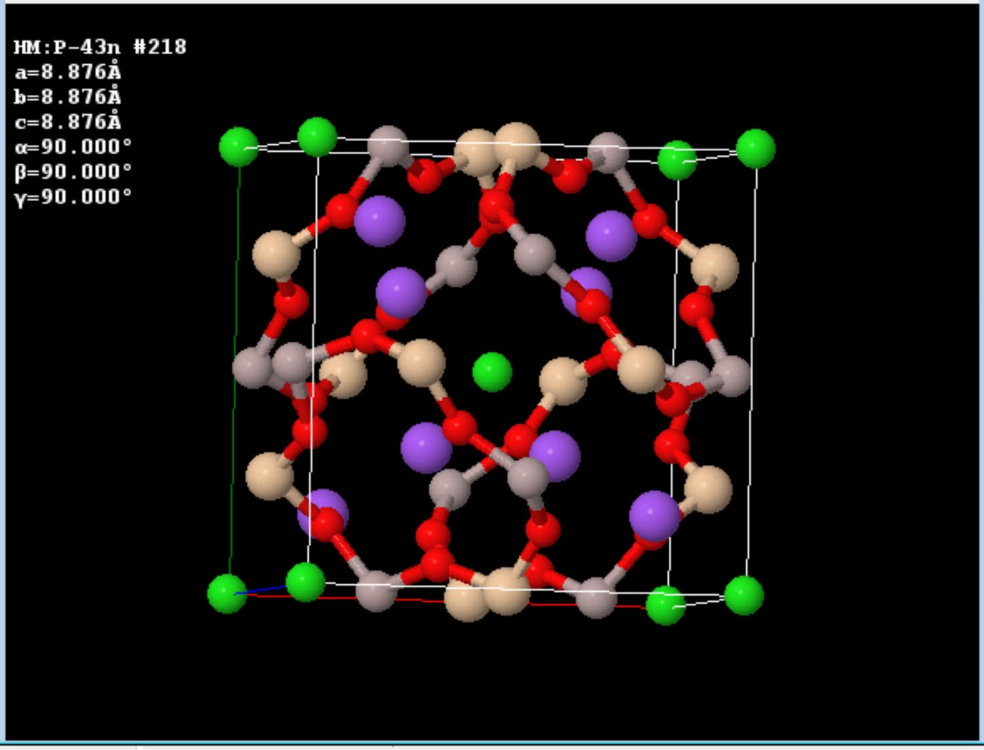
Maximum Combined Bonding Radius: 0% 25% 50% 75% 100% 125% 150%

Subsystem:

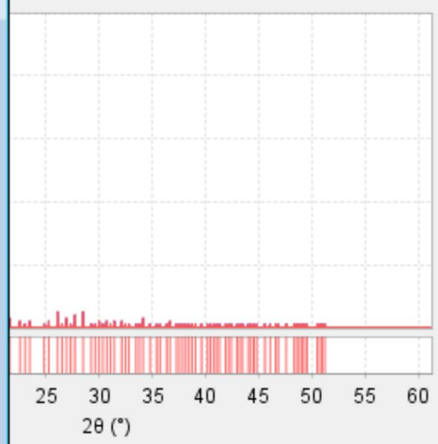
Toggle Modulation

Toggle Animation

Atomic parameters are cross-referenced from PDF entry 04-008-5863



Raw Diffraction Data



Comments

Alternate Name: Sodalite

CAS Number: 1302-90-5

Entry Date: 09/01/1987

Modification Date: - Modifications: -

My Defaults

D3 (Å)	SYS	Auth SPGR	XtlCell a (Å)	XtlCell c (Å)	AuthCell Vol (Å³)	L1
2.380000	C	P-43n	8.890	8.890	702.60	6.2
2.560000	C	P-43n	8.874	8.874	698.81	6.2
1.012000	C	P-43n	8.207	8.207	552.78	4.0
1.918000	C	P-43n	8.150	8.150	541.34	4.0
2.580000	C	I	8.930	8.930	712.12	6.3
1.124000	C	P-43n	8.261	8.261	563.76	3.6
2.560000	X					6.2
6.450000	C	P-43m	9.078	9.078	748.07	9.0
2.872000	C	P-43m	9.090	9.090	751.09	6.4
3.570000	T	I-4	8.583	8.817	649.53	6.1
6.470000	C	P-43n	9.082	9.082	749.11	6.4
2.628000	C		9.100	9.100	753.57	6.4
6.360000	T	I-4	8.975	8.975	722.94	6.3
2.590000	C	P-43n	8.880	8.880	700.23	4.1
2.578000	C		17.709	17.709	5553.70	10.2
2.164000	C	P-43n	9.180	9.180	773.62	6.5
2.461000	C	P-43n	9.220	9.220	783.78	6.5
2.661000	C	P-43n	9.220	9.220	783.78	6.5
2.624000	C	P-43n	9.095	9.095	752.33	6.4
2.081000	C	I-43m	8.824	8.824	687.11	4.4
2.324000	C	P-43n	9.326	9.326	811.12	6.5
4.560000	C	P-43n	9.120	9.120	758.55	6.4
2.148000	C	P-43n	9.117	9.117	757.80	6.4
2.590000	C		8.980	8.980	724.15	6.3
2.409000	C	P-43n	9.011	9.011	731.65	6.3
2.388000	C	P-43n	8.933	8.933	712.84	6.3
2.387000	C	P-43n	8.930	8.930	712.12	6.3
3.615000	T		6.937	8.488	408.46	6.9
2.110000	C	P-43n	8.932	8.932	712.60	6.3
2.580000	C	I	8.921	8.921	709.97	6.3
2.150000	C	P-43n	9.120	9.120	758.53	6.4
2.093000	C	P-43n	8.878	8.878	699.85	6.2
2.110000	C		8.943	8.943	715.24	6.3

[Zeolite

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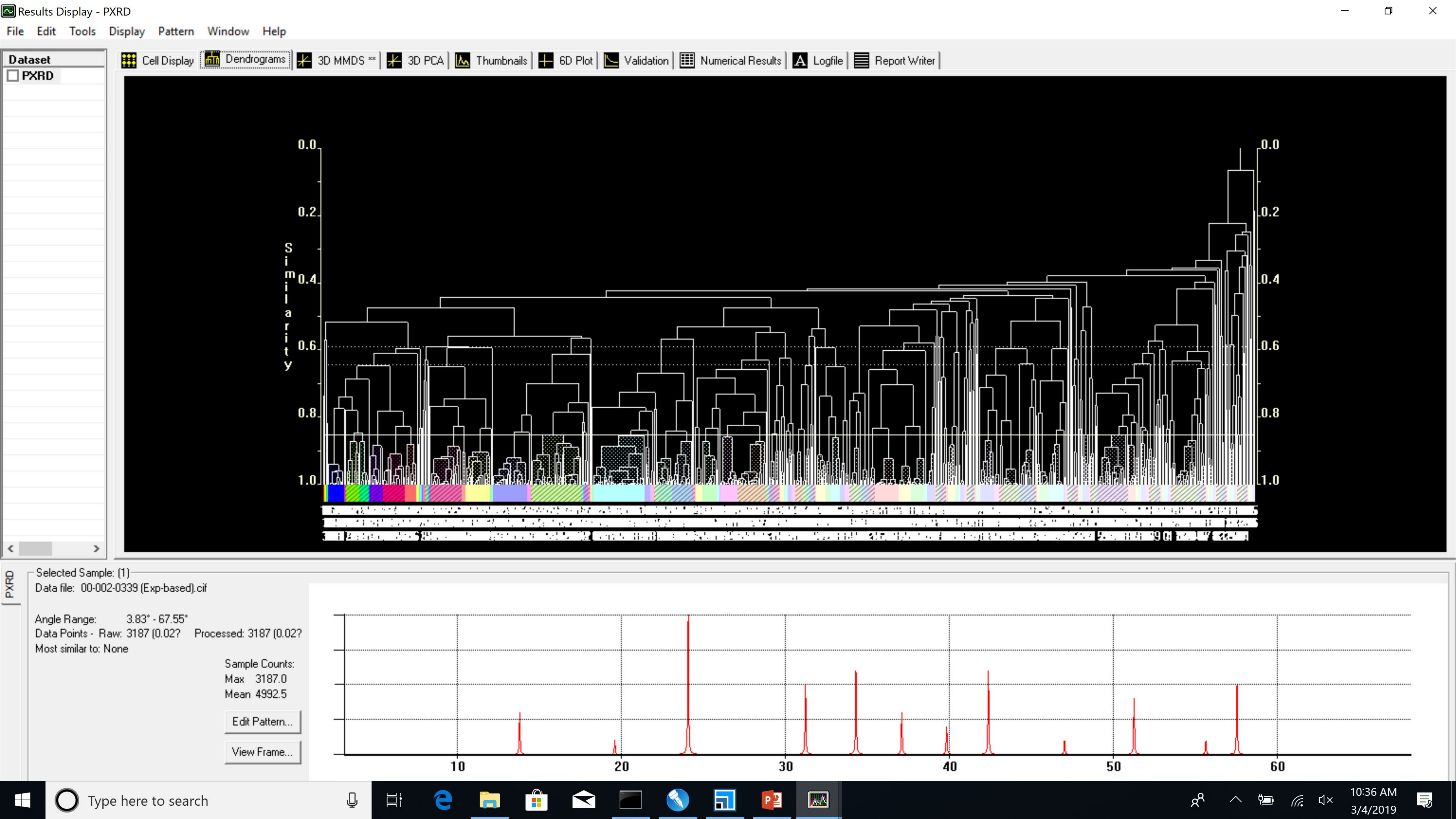
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PXRD
Cell Display
Dendrograms
3D MMDS
3D PCA
Thumbnails
6D Plot
Validation
Numerical Results
Logfile
Report Writer
Similarity
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PXRD
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Data file: 00-002-0339 (Exp-based).cif
Angle Range: 3.83° - 67.55°
Data Points - Raw: 3187 (0.02? Processed: 3187 (0.02?
Most similar to: None
Sample Counts:
Max 3187.0
Mean 4992.5
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View Frame...
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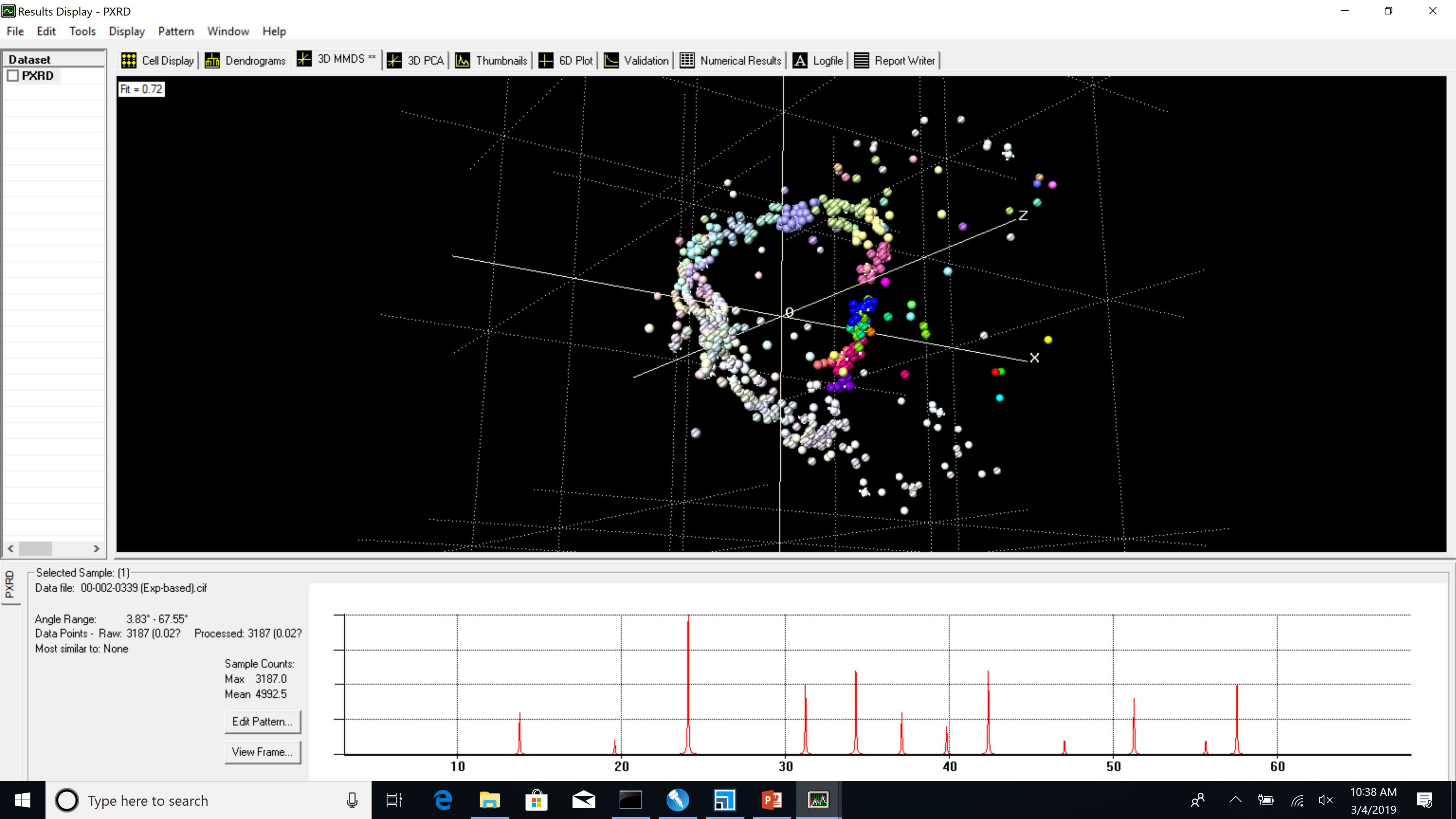
Results Display - PXRD
File Edit Tools Display Pattern Window Help
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Cell Display
Dendrograms
3D MMDS **
3D PCA
Thumbnails
6D Plot
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Numerical Results
Logfile
Report Writer
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PXRD
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Processed: 3187 (0.02?
Most similar to: None
Sample Counts:
Max 3187.0
Mean 4992.5
Edit Pattern...
View Frame...
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3/4/2019

Cluster K5

PDF #	Cation	Framework 1	Framework 2	Framework 3	Extraframework
04-007-7045+	Na	Al	Ge	O	Br
04-017-7142	Na	Al	Ge	O	Br,S
04-009-4300+	Na	Al	Ge	O	Br,OH
04-009-6726+	Na	Al	Si	O	SO_4,H_2O
04-011-7972	Na	Al	Ge	O	NO_2
04-009-5216	Na	Al	Si	O	MnO_4
04-014-4518	Na	Ga	Si	O	I
04-011-7466+	Na,K,Ca	Al	Si	O	SO_4
04-009-5213	Na	Al	Si	O	ClO_4
04-016-7534	Na,K,Ca	Al	Si	O	S,SO_4,Cl,H_2O
04-014-2217	Na	Al	Si	O	MnO_4,OH
04-017-0541+2	Na,Ca	Al	Si	O	SO_4
04-013-1716	Na,K	Al	Si	O	Cl
01-076-8967+	Na	Al	Si	O	SO_4,S_3
01-076-6140	$N(CH_3)_4$	Ga	Ge	O	-

Cluster K

PDF #	Cation	Framework 1	Framework 2	Framework 3	Extraframework
00-038-0022	Na	Al	Si	O	SCN, H_2O
01-073-8449	Na	Al	Si	O	$B(OH)_4$
01-077-1703	Na	Al	Si	O	SO_4, S
04-010-2826	Na	Al	Si	O	SO_4, S
01-085-8449	Na	Al	Si	O	SO_4, Cl
04-009-5214	Na	Al	Si	O	ClO_4
04-009-9801	Na	Al	Si	O	S, H_2O
04-014-8480	Na	Al	Si	O	NO_3
01-072-1614	Na	Al	Si	O	SO_4
04-013-6370	Na	Al	Ge	O	BH_4

The end of the list

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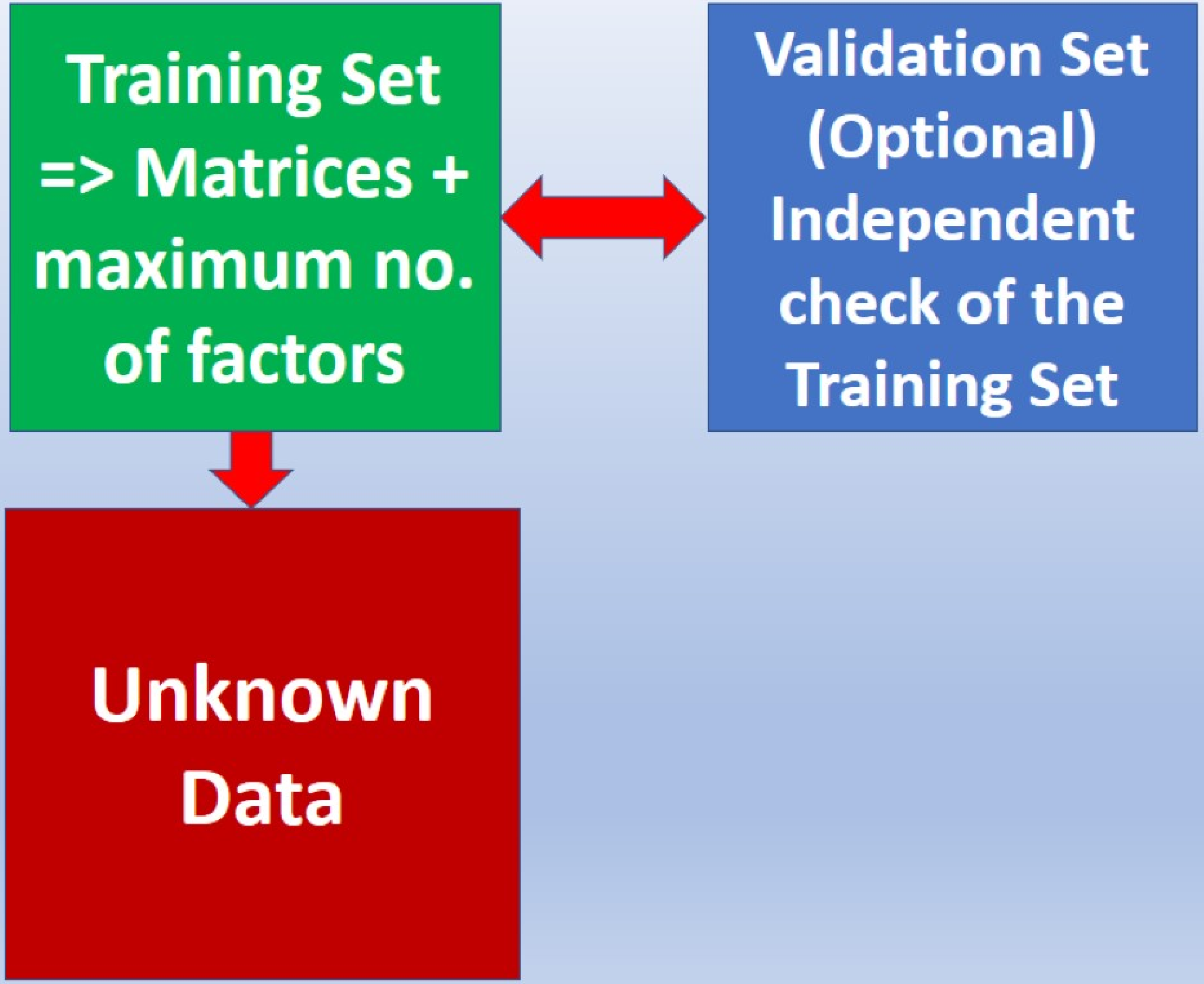
\par Group F7:
\par Sample #  125:\tab 00-050-1699 (Exp-based).cif.
\par Group G7:
\par Sample #  112:\tab 00-047-0597 (Exp-based).cif.
\par Group H7:
\par Sample #   53:\tab 00-041-0072 (Exp-based).cif.
\par Group I7:
\par Sample #   37:\tab 00-035-0002 (Exp-based).cif.
\par Group J7:
\par Sample #    8:\tab 00-016-0612 (Exp-based).cif.
\par Group K7:
\par Sample #   57:\tab 00-041-0535 (Exp-based).cif.
\par Group L7:
\par Sample #   18:\tab 00-024-1045 (Exp-based).cif.
\par Group M8:
\par Sample #   48:\tab 00-039-0191 (Exp-based).cif.
\par Group N8:
\par Sample #   54:\tab 00-041-0073 (Exp-based).cif.
```

Partial Least Squares (PLS) as a Machine Learning Method

Data Sets

- **Training data: {Powder diffraction patterns of mixtures. (Any no. of components in mixture is allowed)} + {Known composition of mixtures}**
- **Validation data: : {Powder diffraction patterns} + {Known compositions}**
- **Unknowns: {Powder diffraction patterns}**

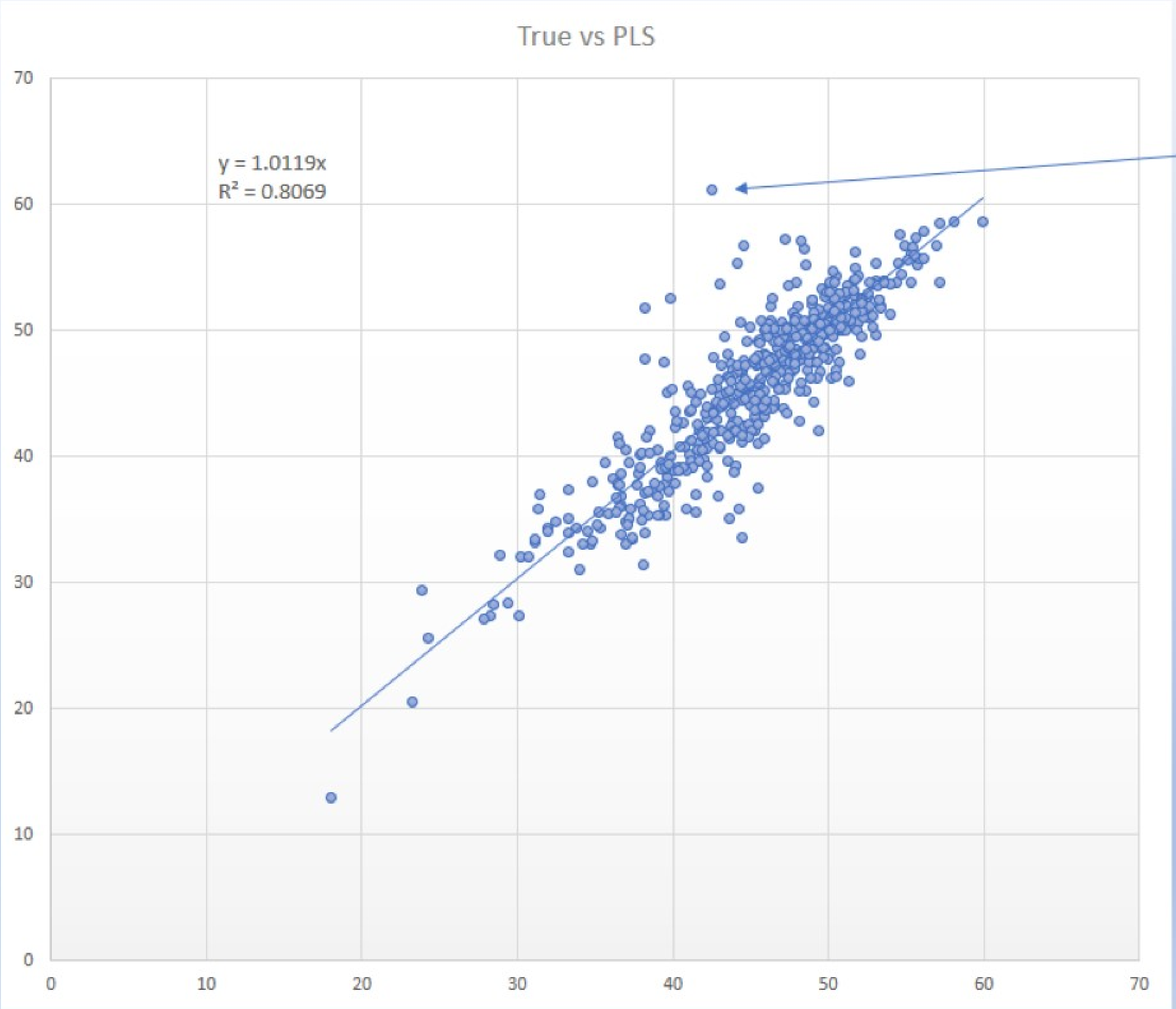

Training Set => Matrices + maximum no. of factors
Validation Set (Optional) Independent check of the Training Set
Unknown Data

PLS on Cement Clinker Data

- **49 training patterns.**
- **44 validation patterns.**
- **538 unknown samples.**
- **18 possible components: AliteM3, AliteM1, sumAlite, Belite, C3ACubic, C3AOrthorhombic ………**

Fast: Training + validation + unknowns takes < 20s on 3yr old laptop with 4 cores.

Gives esds.



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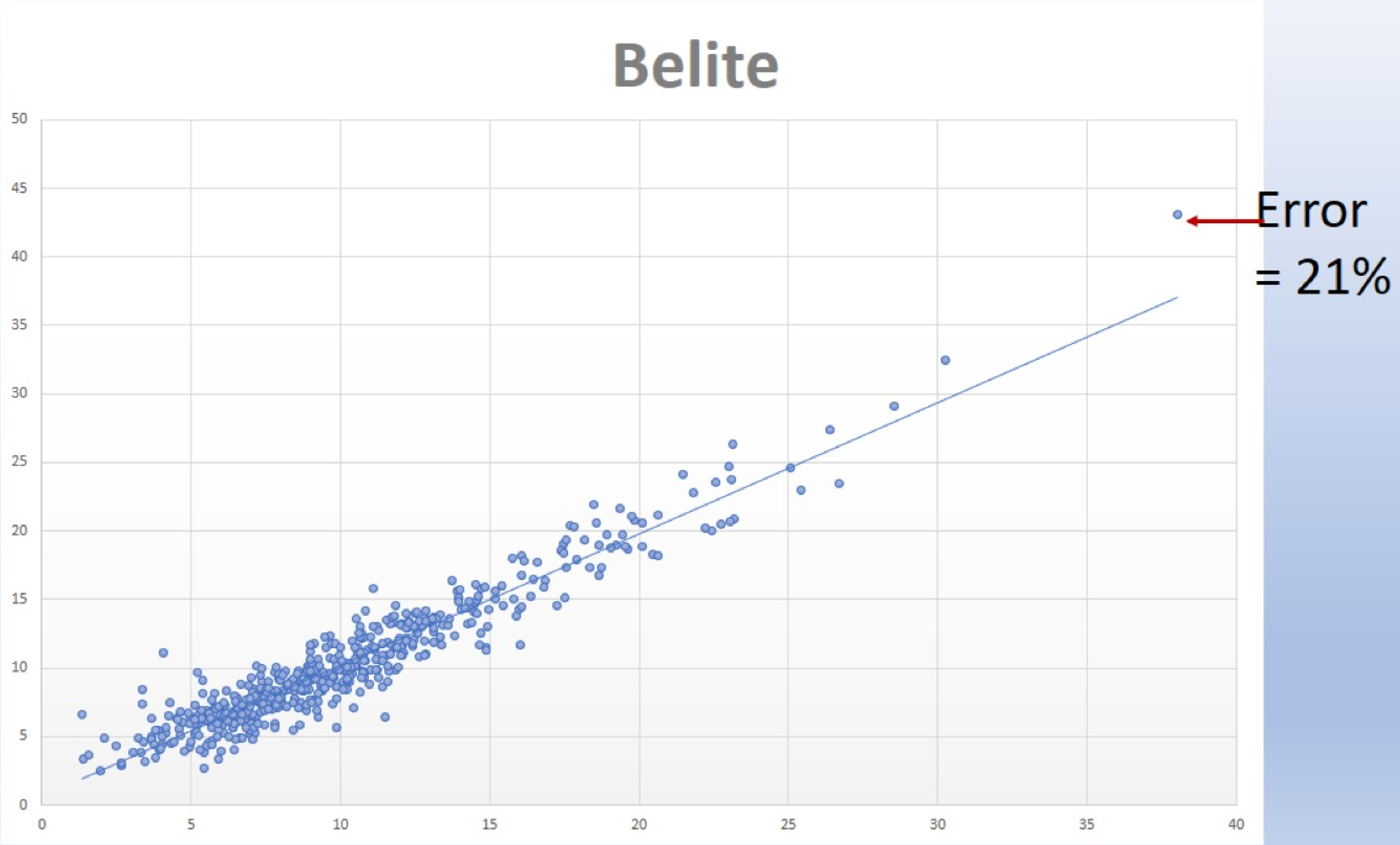
Errors are typically 3-10%

Results for AliteM1


Belite
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Error
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