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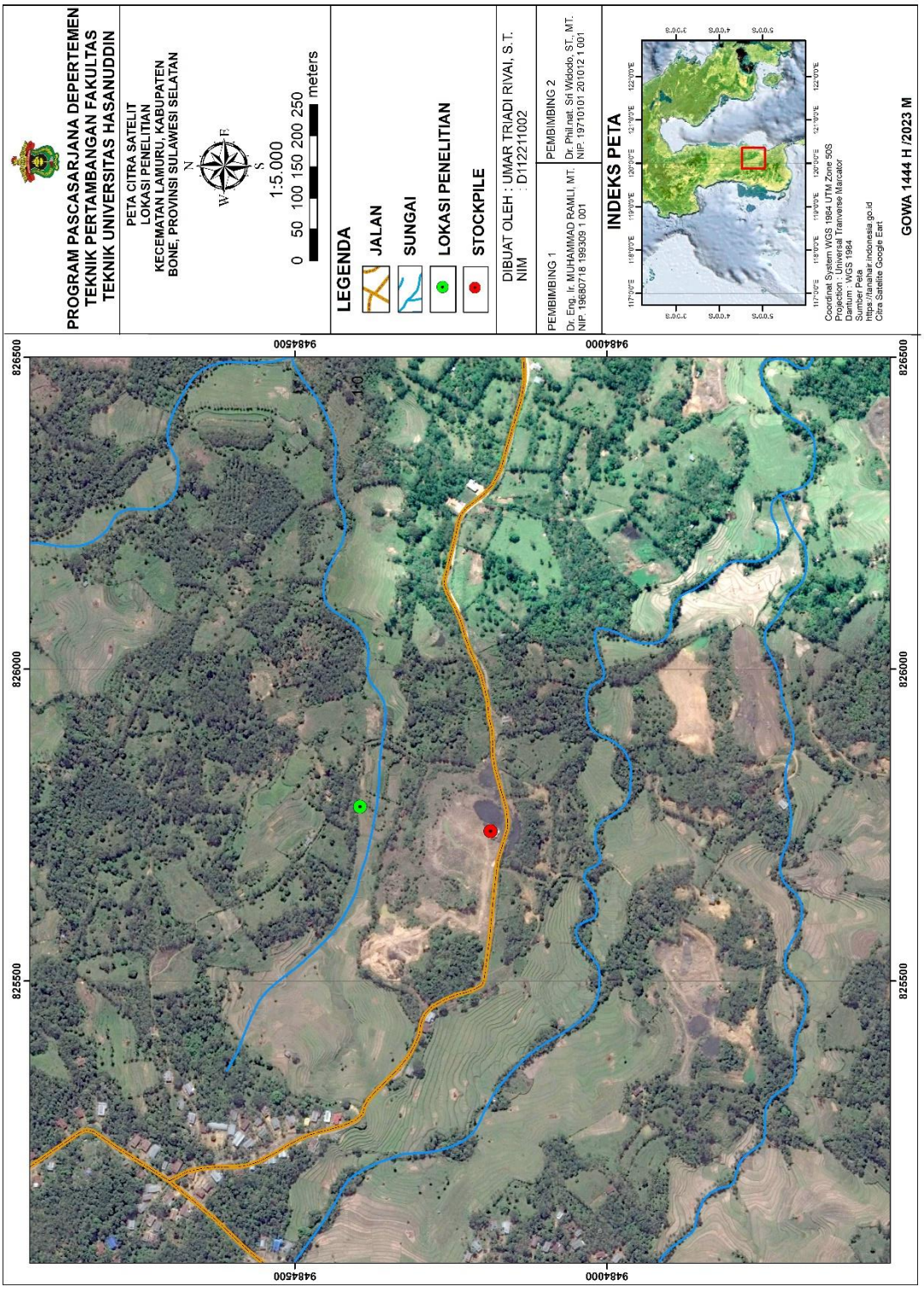
LAMPIRAN

A. PETA TUNJUK LOKASI


PROGRAM PASCASARJANA DEPERTEMEN
TEKNIK PERTAMBANGAN FAKULTAS
TEKNIK UNIVERSITAS HASANUDDIN
PETA CITRA SATELIT
LOKASI PENELITIAN
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LEGENDA
JALAN
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DIBUAT OLEH : UMAR TRIADI RIVAI, S.T.
NIM : D112211002
PEMBIMBING 1
Dr. Eng. Ir. MUHAMMAD RAMLI, MT.
NIP. 196807 18 199309 1 001
PEMBIMBING 2
Dr. Phil.nat. Sri Widodo, ST., MT.
NIP. 19710101 201012 1 001
INDEKS PETA
Coordinat System WGS 1984 UTM Zone 50S
Projection : Universal Tranvelse Mercator
Datum : WGS 1984
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B. HASIL PENGUJIAN LABORATORIUM XRD

Match! Phase Analysis Report

Sample: S1-UTR

Sample Data

File name	S1-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S1-UTR
Data collected	Jun 7, 2022 13:00:08
Data range	5.100° - 70.100°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	0.1°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	28.9	Illite	Al2 H2 K O12 Si4
B	27.6	Calcite	C Ca O3
C	21.2	Quartz	O2 Si
D	20.8	Kaolinite	Al2 O9 Si2
E	1.5	Pyrite	Fe S2
	6.7	*Unidentified peak area*	

A: Illite (28.9 %)

Formula sum	Al2 H2 K O12 Si4
Entry number	96-901-3722
Figure-of-Merit (FoM)	0.477011
Total number of peaks	526
Peaks in range	220
Peaks matched	106
Intensity scale factor	0.15
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.2100 Å b= 9.0200 Å c= 10.1590 Å β= 101.400 °
I/Ic	0.89
Calc. density	2.834 g/cm³
Reference	Drits V. A., Zviagina B. B., McCarty D. K., Salyn A. L., "Factors responsible for crystal-chemical variations in the solid solutionsfrom illite to aluminoceladonite and from glauconite to celadoniteLocality: Ordovician K-bentonite, VermontSample Name: KJMC3", American Mineralogist **95**, 348-361 (2010)

B: Calcite (27.6 %)

Formula sum	C Ca O3
Entry number	96-901-6707
Figure-of-Merit (FoM)	0.832954
Total number of peaks	86
Peaks in range	38
Peaks matched	22
Intensity scale factor	0.51
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9844 Å c= 17.0376 Å
I/Ic	3.10
Calc. density	2.720 g/cm³
Reference	Ondrus P., Veselovsky F., Gabasova A., Hlousek J., Srein V., Vavrnn I., Skala R., Sejkora J., Drabek M., "Primary minerals of the Jachymov ore district", Journal of the Czech Geological Society **48**, 19-147 (2003)

C: Quartz (21.2 %)

Formula sum	O2 Si
Entry number	96-900-9667
Figure-of-Merit (FoM)	0.866801
Total number of peaks	70
Peaks in range	36
Peaks matched	31
Intensity scale factor	0.57
Space group	P 31 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9158 Å c= 5.4091 Å
I/Ic	4.52
Calc. density	2.644 g/cm³
Reference	Gualtieri A. F., "Accuracy of XRPD QPAusing the combined Rietveld-RIR methodLocality: Baveno, Novara, Italy", Journal of Applied Crystallography **33**, 267-278 (2000)

D: Kaolinite (20.8 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.647813
Total number of peaks	528
Peaks in range	250
Peaks matched	133
Intensity scale factor	0.14
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °

Reference:

Entry number: 96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-101-1046;96-901-5000;96-900-1665;96-900-4787;96-900-4919;96-900-7429;96-900-7612;96-900-9523;96-900-9666;96-901-0118;96-901-0494;96-901-0549;96-901-1123;96-901-1745;96-901-1746;96-901-2893;96-901-3719;96-901-3720;96-901-3721;96-901-3722;96-901-3723;96-901-3724;96-901-3733;96-901-3985;96-901-6664

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	12.42	7.1269	254.55	0.7200	D
2	20.00	4.4396	129.44	0.5200	A,D
3	21.02	4.2265	67.61	0.3600	C,D
4	23.24	3.8275	66.19	0.4000	A,B,D
5	25.04	3.5563	47.55	0.5600	D
6	25.04	3.5563	186.64	0.5600	
7	26.82	3.3242	1000.00	0.4463	A,C
8	29.64	3.0140	785.92	0.2549	B,D
9	32.00	2.7969	251.11	0.3951	D
10	33.24	2.6954	118.61	0.1673	A,E
11	35.16	2.5525	216.74	0.4000	A,D
12	36.26	2.4775	206.57	0.4000	A,B,D
13	36.74	2.4462	190.01	0.2409	A,C
14	37.24	2.4145	87.89	0.2993	A,D,E
15	37.94	2.3716	57.38	0.2800	A,D
16	38.56	2.3349	254.01	0.2400	A,D
17	39.62	2.2748	264.93	0.3873	B,C,D
18	40.46	2.2295	85.78	0.2460	A,C,D
19	40.98	2.2024	54.41	0.2667	A,D,E
20	42.64	2.1204	109.28	0.4050	A,C,D
21	43.42	2.0841	113.63	0.2954	A,B
22	46.02	1.9723	104.36	0.6295	C,D
23	47.80	1.9029	186.71	0.4303	A,B,D,E
24	48.82	1.8655	139.95	0.2640	A,B,D
25	50.28	1.8147	258.73	0.2389	A,C,E
26	52.70	1.7369	25.76	0.2800	A
27	55.00	1.6696	70.72	0.2800	A,C,D
28	55.46	1.6568	53.45	0.6400	A,C,D
29	56.44	1.6304	83.23	0.2000	A,B,D,E
30	57.66	1.5987	44.67	0.2400	A,B,D
31	59.28	1.5589	36.39	0.4400	A,D,E
32	60.12	1.5391	196.29	0.2935	A,C,D
33	61.82	1.5008	35.47	1.7600	A,B,D,E
34	62.42	1.4878	63.77	0.3200	A,D
35	64.18	1.4512	21.24	0.2000	A,C,D,E
36	65.14	1.4321	26.17	0.3200	A,B,D
37	66.14	1.4128	26.15	0.2000	B,C,D
38	67.88	1.3808	89.14	0.5200	A,C,D
39	68.44	1.3709	137.65	0.2628	A,C,D
40	69.48	1.3529	30.79	0.2400	A,B,D
41	69.92	1.3454	18.70	0.0916	D

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	126565	100.00%
Background radiation	73830	58.33%
Diffraction peaks	52735	41.67%
Peak area belonging to selected phases	70495	55.70%
Peak area of phase A (Illite)	*20742*	*16.39%*
Peak area of phase B (Calcite)	*13733*	*10.85%*
Peak area of phase C (Quartz)	*15847*	*12.52%*
Peak area of phase D (Kaolinite)	*17946*	*14.18%*
Peak area of phase E (Pyrite)	*2228*	*1.76%*
Unidentified peak area	8515	6.73%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	819	100.00%
Peak intensity belonging to selected phases	519	63.42%
Unidentified peak intensity	300	36.58%

Diffraction Pattern Graphics

I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

E: Pyrite (1.5 %)

Formula sum	Fe S2
Entry number	96-900-0595
Figure-of-Merit (FoM)	0.505740
Total number of peaks	42
Peaks in range	22
Peaks matched	16
Intensity scale factor	0.03
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.4166 Å
I/Ic	3.34
Calc. density	5.014 g/cm³
Reference	Bayliss P., "Crystal structure refinement of a weakly anisotropic pyritecubic model", American Mineralogist **62**, 1168-1172 (1977)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
Bromargyrite	Ag Br	96-901-1686	0.7465
Li In Se2	In Li Se2	96-810-3912	0.7196
	As0.5 Li0.5 Se	96-410-2046	0.7195
Sodium	Na	96-901-1003	0.7107
	La0.1 Mn O2.5 Sr0.9	96-400-1124	0.7067
Halite	Cl Na	96-900-6370	0.7047
Calcium carbonate (Calcite)	Ca C O3	96-101-0963	0.7024
Halite	Cl Na	96-900-6371	0.6992
(Pd23 Pr2)0.08	Pd1.84 Pr0.16	96-154-0759	0.6983
	Cl K0.6 Na0.4	96-900-3188	0.6935
	Cl K0.6 Na0.4	96-900-3212	0.6935
	Cl K0.6 Na0.4	96-900-3185	0.6918
Calcium carbonate (Calcite)	Ca C O3	96-101-0929	0.6886
Halite	Cl Na	96-900-6372	0.6885
Nitrogen	N2	96-901-2479	0.6884
Digenite	Cu1.8 S	96-900-0118	0.6876
(Gd0.75 Mg0.25)	Gd0.75 Mg0.25	96-152-2529	0.6868
Li0.026 Ti O2	Li0.026 O2 Ti	96-412-4519	0.6863
La Tl	La Tl	96-152-3873	0.6854
	Cl K0.5 Na0.5	96-900-3217	0.6852
Calcite	C Ca O3	96-901-6707	0.6851
Cu1.78 S	Cu1.78 S	96-152-8227	0.6846
(Sr0.84 La0.16) (Ru O3)	La0.16 O3 Ru Sr0.84	96-153-7566	0.6842
	O7 P2 Sn	96-591-0165	0.6838
	Cl K0.6 Na0.4	96-900-3194	0.6821
	Cl K0.6 Na0.4	96-900-3198	0.6820
	Cl K0.6 Na0.4	96-900-3213	0.6820
	Cl K0.6 Na0.4	96-900-3205	0.6818
Ba Pb0.74 Sb0.2 Bi0.057 O3	Ba Bi0.057 O3 Pb0.74 Sb0.2	96-810-3948	0.6817
	C Ca O3	96-210-0190	0.6812
(La0.83 Sr0.17) Ru O2.94	La0.83 O2.94 Ru Sr0.17	96-153-7565	0.6810
(Sr0.76 La0.24) Ru0.96 O2.7	La0.24 O2.7 Ru0.96 Sr0.76	96-153-7567	0.6807
Digenite	Cu1.84 S	96-901-5841	0.6794
	Cl K0.6 Na0.4	96-900-3216	0.6783
silver germanium antimony telluride	Ag0.133 Ge0.533 Sb0.267 Te	96-434-0363	0.6781
	C Cu N	96-110-0001	0.6779
	C Cu N	96-110-1019	0.6779
Po Br4	Br4 Po	96-154-1437	0.6778
Titanium oxide (Anatase)	Ti O2	96-500-0224	0.6774
Eu Ba2 Nb O5.5	Ba2 Eu Nb O5.5	96-434-3689	0.6773
	I6 Na2 O18 Ti	96-410-4386	0.6772
Ba (Fe0.34 Ho0.33 U0.33 O3)	Ba Fe0.34 Ho0.33 O3 U0.33	96-152-7443	0.6753
Sr2 (Fe1.5 Mo0.5) O6	Fe1.5 Mo0.5 O6 Sr2	96-153-1826	0.6749
Ba (Pb0.7 Sb0.25 Bi0.05) O3	Ba Bi0.05 O3 Pb0.7 Sb0.25	96-810-4408	0.6739
Cd.5 Bi1.5 O2.75	Bi1.5 Cd0.5 O2.75	96-153-9108	0.6736
Wakefieldite-(Y)	O2 V Y	96-901-6009	0.6733
Anatase	O2 Ti	96-900-8215	0.6732
Fergusonite-(Y)	Nb O4 Y0.85 Yb0.15	96-901-1839	0.6730
Sr2 (Fe1.4 Mo0.6) O6	Fe1.4 Mo0.6 O6 Sr2	96-153-1829	0.6727
CaCO3	C Ca O3	96-702-0140	0.6726
(Ag Bi) (Se0.98 Te1.02)	Ag Bi Se0.98 Te1.02	96-150-9242	0.6724
Manganese carbonate (Rhodochrosite)	Mn O3	96-101-1229	0.6718

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.40
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
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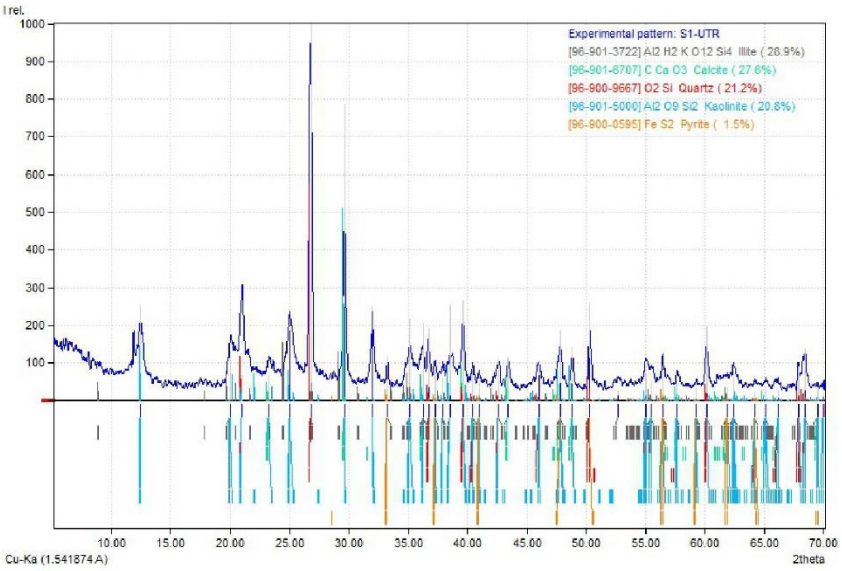
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user



Match! Phase Analysis Report

Sample: S2-UTR

Sample Data

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Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	40.8	Quartz	O2 Si
B	29.9	Kaolinite	Al2 O9 Si2
C	16.5	Calcite	C Ca O3
D	12.7	Pyrite	Fe S2
	9.1	*Unidentified peak area*	

A: Quartz (40.8 %)

Formula sum	O2 Si
Entry number	96-900-5018
Figure-of-Merit (FoM)	0.839318
Total number of peaks	70
Peaks in range	36
Peaks matched	28
Intensity scale factor	0.41
Space group	P 32 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9137 Å c= 5.4047 Å
I/Ic	2.99
Calc. density	2.649 g/cm³
Reference	Kihara K., "An X-ray study of the temperature dependence of the quartz structureSample: at T = 298 K", European Journal of Mineralogy **2**, 63-77 (1990)

B: Kaolinite (29.9 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.621173
Total number of peaks	528
Peaks in range	240
Peaks matched	109
Intensity scale factor	0.12
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

C: Calcite (16.5 %)

Formula sum	C Ca O3
Entry number	96-901-5067
Figure-of-Merit (FoM)	0.764172
Total number of peaks	86
Peaks in range	36
Peaks matched	15
Intensity scale factor	0.18
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9769 Å c= 17.3479 Å
I/Ic	3.18
Calc. density	2.680 g/cm³
Reference	Antao S. M., Hassan I., "Temperature dependence of the structural parametersin the transformation of aragonite to calcite,as determined from in situ synchrotron powder X-ray-diffraction dataNote: T = 556 CNote: P = 101 kPa", The Canadian Mineralogist **48**, 1225-1236 (2010)

D: Pyrite (12.7 %)

Formula sum	Fe S2
Entry number	96-900-0595
Figure-of-Merit (FoM)	0.673592
Total number of peaks	42
Peaks in range	20
Peaks matched	15
Intensity scale factor	0.14
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.4166 Å
I/Ic	3.34
Calc. density	5.014 g/cm³
Reference	Bayliss P., "Crystal structure refinement of a weakly anisotropic pyritecubic model", American Mineralogist **62**, 1168-1172 (1977)

Candidates

Name	Formula	Entry No.	FoM
	Pd	96-151-2532	0.6842
	Cl6 H12 N4 Pt Sn	96-200-9768	0.6964
	O2 Si	96-210-0189	0.7489
	Al C0.47 Co2.04 O9	96-210-2794	0.7339
	O2 Si	96-230-0371	0.7463
	Cu3 Fe4 O12 Y	96-411-9596	0.7207
	H13 O15 U3	96-430-6723	0.6831
	H0.9 Na0.22 O2.45 Ru	96-431-0643	0.7427
	Cl16 Nb10 O7	96-431-2742	0.7189
	Cs2 O8 V3	96-433-4973	0.6794
	Cu3 Fe4 Ho O12	96-433-6918	0.6922
	Cu3 Er Fe4 O12	96-433-6919	0.6872
	Cu3 Fe4 O12 Tm	96-433-6920	0.6834
	Cu3 Fe4 O12 Yb	96-433-6921	0.6788
	Ag Cu3 O12 V4	96-433-7058	0.7107
	Ca Cu2.79 Fe4.21 O12	96-434-4870	0.7216
	C Ca O3	96-450-2444	0.6860
	O7 P2 Si	96-591-0161	0.7350
	F Na Nb6 O15	96-591-0193	0.7021
	Ge O7 P2	96-591-0254	0.7330
	O2 Si	96-710-3015	0.7490
	Al0.05 Li0.05 O2 Si0.95	96-900-2384	0.6837
	B N	96-900-8998	0.7760
	Cl Fe O	96-900-9192	0.7418
	Cs2 H9.5 O37.75 Se4 U7	96-901-4848	0.7192
	N2 O13 P4 Si	96-901-6169	0.7597
(Au Zn19)0.1	Au0.1 Zn1.9	96-151-0412	0.6859
(B Fe20 Y2)0.088	B0.086 Fe1.74 Y0.174	96-151-1463	0.6793
(Co1.5 Ir0.5)	Co1.5 Ir0.5	96-152-4149	0.7007
(Co1.5 Rh0.5)	Co1.5 Rh0.5	96-152-4156	0.7002
(Co3 Ir7)0.2	Co1.4 Ir0.6	96-152-4897	0.7020
(Cu0.85 Ge0.15)	Cu0.85 Ge0.15	96-152-4232	0.7059
(Dy0.1 Pd0.9)	Dy0.1 Pd0.9	96-152-4817	0.6848
(Er0.11 Pd0.89)	Er0.11 Pd0.89	96-152-4816	0.6844
(Gd0.5 Nd0.5) Zn	Gd0.5 Nd0.5 Zn	96-152-3172	0.7158
(Hf0.08 Pu0.92)	Hf0.08 Pu0.92	96-152-2482	0.7472
(Ho0.12 Pd0.88)	Ho0.12 Pd0.88	96-152-2389	0.6844
(In3 Pd17)0.2	In0.6 Pd3.4	96-153-7912	0.6800
(Pb0.12 Pd0.88)	Pb0.12 Pd0.88	96-152-3554	0.6824
(Pd0.5 Rh0.5)3 Zr	Pd1.5 Rh1.5 Zr	96-152-2724	0.6811
(Pd0.83 Sn0.17)	Pd0.83 Sn0.17	96-152-2086	0.6804
(Pd0.845 Zr0.155)	Pd0.845 Zr0.155	96-152-2600	0.6818
(Pd17 Sn3)0.2	Pd3.4 Sn0.6	96-153-7916	0.6791
(Pd4 Zr)0.8	Pd3.184 Zr0.816	96-153-7661	0.6848
(Pd9 Y)0.4	Pd3.6 Y0.4	96-153-8636	0.6852
(Pu0.8 Zr0.2)	Pu0.8 Zr0.2	96-152-2481	0.7413
(Ti2 D3)1.6	D3.4 Ti4	96-152-5008	0.7170
Afwillite	Ca3 H6 O10 Si2	96-900-7429	0.3979
Afwillite	Ca3 H6 O10 Si2	96-900-7612	0.3963
Afwillite	Ca3 H6 O10 Si2	96-901-3985	0.3865
Ag Dy	Ag Dy	96-150-9296	0.7008
Ag Gd	Ag Gd	96-150-9361	0.7347
and 150 others...			

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number: 96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-1665;96-900-4787;96-900-4919;96-900-7429;96-900-7612;96-900-9523;96-900-9666;96-901-0118;96-901-0494;96-901-0549;96-901-1123;96-901-1745;96-901-1746;96-901-2893;96-901-3719;96-901-3720;96-901-3721;96-901-3722;96-901-3723;96-901-3724;96-901-3733;96-901-3985;96-901-6664;96-101-1046;96-901-5000

Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	11.84	7.4747	441.66	0.7610	
2	12.30	7.1962	4.86	0.5854	B
3	12.34	7.1729	0.00	0.2659	
4	19.90	4.4617	53.09	0.3375	B
5	20.80	4.2707	330.15	0.9766	A,B
6	23.38	3.8049	73.57	0.4800	C

7	23.40	3.8017	163.16	0.4800	B
8	24.98	3.5647	262.89	0.4400	B
9	25.02	3.5591	111.53	0.3600	
10	25.08	3.5507	83.55	0.5600	B
11	26.74	3.3339	1000.00	0.3450	A
12	29.18	3.0605	243.30	1.0662	C
13	29.50	3.0280	302.51	0.1544	B
14	33.12	2.7049	327.33	0.2745	D
15	35.04	2.5609	119.71	1.4400	B
16	36.10	2.4881	87.74	1.4400	B,C
17	36.62	2.4540	37.12	1.4400	A
18	37.18	2.4183	107.36	0.1931	B,D
19	37.90	2.3740	74.33	1.8972	B
20	38.58	2.3337	116.02	0.3561	B
21	39.52	2.2803	132.83	0.3334	A,B,C
22	40.32	2.2369	35.67	0.1330	A,B
23	40.80	2.2117	111.38	0.4280	B,D
24	42.50	2.1271	67.26	0.8800	A,B
25	43.00	2.1035	29.56	0.8800	B
26	43.40	2.0850	88.27	0.2067	C
27	45.92	1.9763	180.29	0.5060	A,B
28	47.50	1.9142	90.26	1.1878	B,D
29	48.44	1.8792	57.11	0.5465	B,C
30	50.26	1.8154	227.04	0.3173	A,D
31	54.94	1.6713	83.61	0.2800	A,B
32	56.32	1.6336	127.48	0.7296	B,D
33	56.86	1.6193	42.15	0.0953	B,C
34	59.96	1.5428	96.31	0.3298	A
35	61.78	1.5017	61.11	0.4000	B,D
36	62.34	1.4895	86.03	0.3588	B
37	64.30	1.4488	35.41	0.9517	A,B,C,D
38	67.78	1.3826	59.19	0.2400	A,B
39	68.36	1.3723	89.39	0.4144	A,B

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

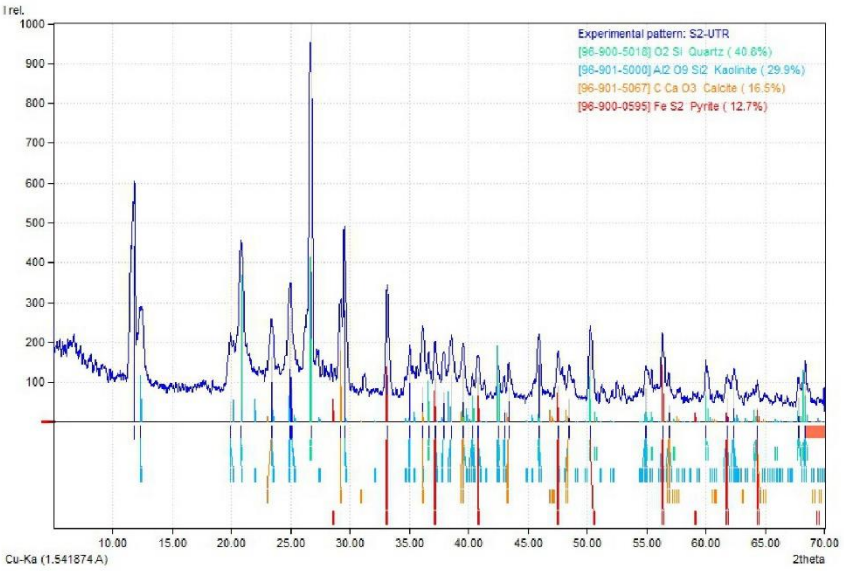
Based on calculated profile

Profile area	*Counts*	*Amount*
Overall diffraction profile	137289	100.00%
Background radiation	83838	61.07%
Diffraction peaks	53451	38.93%
Peak area belonging to selected phases	65206	47.50%
Peak area of phase A (Quartz)	*29343*	*21.37%*
Peak area of phase B (Kaolinite)	*16799*	*12.24%*
Peak area of phase C (Calcite)	*7684*	*5.60%*
Peak area of phase D (Pyrite)	*11380*	*8.29%*
Unidentified peak area	12471	9.08%

Peak Residuals

Peak data	*Counts*	*Amount*
Overall peak intensity	1182	100.00%
Peak intensity belonging to selected phases	502	42.48%
Unidentified peak intensity	680	57.52%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S3-UTR

Sample Data

File name	S3-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S3-UTR
Data collected	Jun 7, 2022 13:00:09
Data range	5.020° - 70.020°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	0.02°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	33.5	Quartz	O2 Si
B	22.7	Kaolinite	Al2 O9 Si2
C	21.1	Chlorite	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
D	17.9	Illite	Al2 H2 K O12 Si4
E	2.3	Arsenopyrite	As Fe S
F	2.2	Calcite	C Ca O3
G	0.3	Pyrite	Fe S2
	5.2	*Unidentified peak area*	

A: Quartz (33.5 %)

Formula sum	O2 Si
Entry number	96-901-2601
Figure-of-Merit (FoM)	0.845875
Total number of peaks	70
Peaks in range	36
Peaks matched	31
Intensity scale factor	0.65
Space group	P 31 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9140 Å c= 5.4060 Å
I/Ic	4.74
Calc. density	2.648 g/cm³
Reference	Hazen R. M., Finger L. W., Hemley R. J., Mao H. K., "High-pressure crystal chemistry and amorphization of alpha-quartzLocality: syntheticSample: P = 1 bar", Solid State Communications **72**, 507-511 (1989)

B: Kaolinite (22.7 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.713343
Total number of peaks	528
Peaks in range	240
Peaks matched	128
Intensity scale factor	0.11
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

C: Chlorite (21.1 %)

Formula sum	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
Entry number	96-901-0167
Figure-of-Merit (FoM)	0.396943
Total number of peaks	600
Peaks in range	305
Peaks matched	129
Intensity scale factor	0.07
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.2930 Å b= 9.1680 Å c= 14.1900 Å β= 96.790 °
I/Ic	0.85
Calc. density	2.777 g/cm³
Reference	Zanazzi P. F., Montagnoli M., Nazzareni S., Comodi P., "Structural effects of pressure on monoclinic chlorite: a single-crystal studyLocality: Alpe Raguzzolo, Val Malenco, Italy Sample: P = 2.28 GPa", American Mineralogist **92**, 655-661 (2007)

D: Illite (17.9 %)

Formula sum	Al2 H2 K O12 Si4
Entry number	96-901-3723
Figure-of-Merit (FoM)	0.612792
Total number of peaks	526
Peaks in range	212
Peaks matched	117
Intensity scale factor	0.07
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.2350 Å b= 9.0320 Å c= 10.1400 Å β= 101.520 °

I/Ic	0.89
Calc. density	2.822 g/cm³
Reference	Drits V. A., Zviagina B. B., McCarty D. K., Salyn A. L., "Factors responsible for crystal-chemical variations in the solid solutionsfrom illite to aluminoceladonite and from glauconite to celadoniteLocality: South Urals, RussiaSample Name: 60", American Mineralogist **95**, 348-361 (2010)

E: Arsenopyrite (2.3 %)

Formula sum	As Fe S
Entry number	96-210-4742
Figure-of-Merit (FoM)	0.445315
Total number of peaks	410
Peaks in range	172
Peaks matched	68
Intensity scale factor	0.02
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 5.7434 Å b= 5.6698 Å c= 5.7871 Å α= 90.000° β= 112.191 ° γ= 90.000 °
I/Ic	2.30
Calc. density	6.198 g/cm³
Reference	Elliot Alexander Dean, "Structure of pyrrhotite 5C (Fe~9~S~10~)", , 1448-1469 (1961)

F: Calcite (2.2 %)

Formula sum	C Ca O3
Entry number	96-901-5074
Figure-of-Merit (FoM)	0.627903
Total number of peaks	86
Peaks in range	36
Peaks matched	15
Intensity scale factor	0.03
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9759 Å c= 17.4486 Å
I/Ic	3.12
Calc. density	2.665 g/cm³
Reference	Antao S. M., Hassan I., "Temperature dependence of the structural parametersin the transformation of aragonite to calcite,as determined from in situ synchrotron powder X-ray-diffraction dataNote: T = 681 CNote: P = 101 kPa", The Canadian Mineralogist **48**, 1225-1236 (2010)

G: Pyrite (0.3 %)

Formula sum	Fe S2
Entry number	96-901-5843
Figure-of-Merit (FoM)	0.469155
Total number of peaks	32
Peaks in range	18
Peaks matched	13
Intensity scale factor	0.00
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.4140 Å
I/Ic	3.10
Calc. density	5.022 g/cm³
Reference	Oftedal I., "Uber die Kristallstrukturen der verbindungen RuS2, OsS2, MnTe2 und AuSb2.Mit einem Anhang uber die Gitterkonstant von Pyrit", Zeitschrift fur Physikalische Chemie **135**, 291-299 (1928)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
Ta	Ta	96-154-1267	0.7404
	Nb	96-400-0949	0.7394
Niobium	Nb	96-900-8547	0.7385
(Nb Ta)	Nb Ta	96-152-3087	0.7378
Rh Zr	Rh Zr	96-154-0936	0.7378
Villiaumite	F Na	96-900-7463	0.7358
Na2 (S2 O3)	Na2 O3 S2	96-722-2828	0.7337
Ag2 Te	Ag2 Te	96-150-9724	0.7325
Ag Cd	Ag Cd	96-150-9174	0.7316
(Ga0.15 Nb0.85)	Ga0.15 Nb0.85	96-152-3937	0.7312
(Cr0.15 Ta0.85)	Cr0.15 Ta0.85	96-152-7975	0.7310
Nb Ta	Nb Ta	96-153-7943	0.7228
Dickite	Al2 H4 O9 Si2	96-900-3082	0.7209
Na.5 Zr6 C Cl15	C Cl15 Na0.5 Zr6	96-153-1026	0.7177
	Ga3 H13 Li2 O24 Te6	96-431-7358	0.7175
	Ag2 Li Sn	96-720-4712	0.7149
Dickite	Al2 H4 O9 Si2	96-900-0123	0.7135
Calcium sulfate dihydrate (Gypsum)	Ca H4 O6 S	96-101-1075	0.7133
Dickite	Al2 H4 O9 Si2	96-901-3940	0.7133
Villiaumite	F Na	96-900-7462	0.7131
Villiaumite	F Na	96-900-7461	0.7117
Rh Zr	Rh Zr	96-152-3580	0.7049
Na (P F6)	F6 Na P	96-152-1417	0.7047
Dickite	Al2 H4 O9 Si2	96-901-3920	0.7044
Tetracalcium dialuminium dodecahydroxide carbonate pentahydrate	Al2 Ca4 H22 O20	96-100-0460	0.7042
Richetite	Fe0.47 H24 Mg0.83 O173 Pb8.74 U36	96-900-4468	0.6997
Au Sn Tm	Au Sn Tm	96-151-0304	0.6996
Zn Zr	Zn Zr	96-152-7719	0.6992
Brushite (deuterated)	Ca D5 O6 P	96-900-7309	0.6990
Nb	Nb	96-153-9042	0.6986
Titanium-beta	Ti	96-900-8555	0.6986
Tantalum	Ta	96-900-8553	0.6985
Brushite (deuterated)	Ca D5 O6 P	96-900-7310	0.6973
(Ga Sb)0.5	Ga0.5 Sb0.5	96-152-3073	0.6959

Cu2 Ho In	Cu2 Ho In	96-152-4285	0.6951
Carbonated calcium hemicarboaluminate	C0.4 Al Ca2 O9.2	96-210-5252	0.6925
Li Ag1.86 In1.14	Ag1.86 In1.14 Li	96-150-9615	0.6923
Villiaumite	F Na	96-900-7464	0.6922
Ag Li2 Sb	Ag Li2 Sb	96-150-9446	0.6920
Li2 (Ag Sb)	Ag Li2 Sb	96-150-9447	0.6906
Larisaite	H22 K0.15 Na1.2 O38 Se4 U6	96-900-5675	0.6895
Nb Ti	Nb Ti	96-153-8067	0.6881
(Au Nb3)0.5	Au0.5 Nb1.5	96-151-0259	0.6878
(H3 O)4 (Ge7 O16) (H2 O)3	Ge7 H18 O23	96-153-3323	0.6875
Li0.026 Ti O2	Li0.026 O2 Ti	96-412-4519	0.6875
Hessite	Ag2 Te	96-900-8422	0.6852
Au Er Sn	Au Er Sn	96-151-0130	0.6839
Titanium bis(hydrogenphosphate(V)) hydrate - $-alpha	H4 O9 P2 Ti	96-100-6112	0.6838
Sophiite	Cl2 O3 Se Zn2	96-901-1799	0.6837
(Pd0.37 Zr0.63)	Pd0.37 Zr0.63	96-152-2585	0.6832
Hexarhenium octaselenide dibromide	Br2 Re6 Se8	96-100-8848	0.6819
	Br Re3 Se4	96-901-6433	0.6819

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number:

96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-1665;96-900-4787;96-900-4919;96-900-7429;96-900-7612;96-900-9523;96-900-9666;96-901-0118;96-901-0494;96-901-0549;96-901-1123;96-901-1745;96-901-1746;96-901-2893;96-901-3719;96-901-3720;96-901-3721;96-901-3722;96-901-3723;96-901-3724;96-901-3733;96-901-3985;96-901-6664;96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707;96-101-1046;96-901-5000;96-201-4618;96-201-4619;96-201-4931;96-220-5377;96-220-7380;96-220-7381;96-901-0164;96-901-0165;96-901-0166;96-901-0167;96-901-0168;96-901-0169;96-901-0170

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	6.84	12.9276	28.75	0.2800	
2	11.36	7.7897	45.52	0.2800	
3	11.55	7.6620	254.45	0.2800	
4	11.71	7.5587	261.64	0.2800	
5	11.88	7.4496	67.49	0.2800	
6	12.27	7.2166	155.02	0.2800	
7	12.44	7.1155	96.24	0.2800	B
8	12.59	7.0300	62.93	0.2800	C
9	19.86	4.4702	136.24	0.2800	B,C,D
10	20.00	4.4407	84.87	0.2800	
11	20.10	4.4178	56.10	0.2800	B
12	20.26	4.3837	71.21	0.2800	B,D
13	20.45	4.3432	83.54	0.2800	C,D
14	20.90	4.2498	356.48	0.2800	A,B
15	21.10	4.2106	94.63	0.2800	C
16	21.26	4.1794	42.67	0.2800	
17	21.40	4.1532	63.14	0.2800	
18	21.52	4.1294	48.14	0.2800	D
19	21.70	4.0955	36.42	0.2800	D
20	21.92	4.0549	43.41	0.2800	B
21	22.22	4.0008	43.04	0.2800	C
22	22.58	3.9373	34.01	0.2800	
23	22.91	3.8819	32.24	0.2800	C,E,F
24	23.40	3.8014	106.47	0.2800	C,D
25	23.50	3.7853	32.52	0.2800	B
26	23.89	3.7251	32.65	0.2800	
27	24.30	3.6634	40.86	0.2800	C,D,E
28	24.50	3.6334	43.88	0.2800	D
29	24.99	3.5639	223.43	0.2800	B
30	25.12	3.5452	51.95	0.2800	
31	25.28	3.5231	72.73	0.2800	B,C
32	25.48	3.4959	61.87	0.2800	
33	25.76	3.4583	36.94	0.2800	C
34	26.00	3.4275	31.54	0.2800	
35	26.73	3.3347	1000.00	0.2800	A,D
36	27.53	3.2400	33.55	0.2800	B
37	28.37	3.1458	31.02	0.2800	G
38	28.74	3.1067	33.02	0.2800	C,G

39	28.95	3.0846	37.86	0.2800	
40	29.22	3.0561	122.60	0.2800	D,F
41	31.23	2.8637	28.58	0.2800	E
42	31.26	2.8614	5.66	0.2800	E
43	33.32	2.6887	32.36	0.2800	D,E,G
44	34.98	2.5653	120.35	0.2800	B,C,D,E
45	35.15	2.5535	61.86	0.2800	C,E
46	35.32	2.5413	35.23	0.2800	B,E
47	35.49	2.5294	66.15	0.2800	B,C
48	35.76	2.5107	46.17	0.2800	C,E
49	35.99	2.4958	69.88	0.2800	D,E
50	36.11	2.4873	32.34	0.2800	B,D,F
51	36.32	2.4736	35.75	0.2800	D
52	36.61	2.4548	127.19	0.2800	A,D
53	36.78	2.4437	50.14	0.2800	D,E
54	37.19	2.4177	32.15	0.2800	B,C,D,E,G
55	37.80	2.3802	58.91	0.2800	B,C,E
56	37.94	2.3715	33.78	0.2800	C,D
57	38.14	2.3597	35.86	0.2800	C
58	38.36	2.3464	76.11	0.2800	B,C,D
59	38.62	2.3316	89.82	0.2800	
60	38.78	2.3221	37.56	0.2800	
61	38.96	2.3120	33.03	0.2800	
62	39.25	2.2953	55.87	0.2800	C
63	39.41	2.2866	43.73	0.2800	A,C,F
64	39.58	2.2772	77.47	0.2800	A,B,C,D
65	40.37	2.2344	63.00	0.2800	A,B,C,D
66	40.71	2.2166	37.43	0.2800	B,C,D,E,G
67	42.52	2.1263	87.54	0.2800	A,B,C,D,E
68	45.24	2.0045	29.96	0.2800	B,C,D,E
69	45.52	1.9929	35.74	0.2800	B,C,D
70	45.85	1.9792	79.53	0.2800	A,B,C,D,E
71	47.89	1.8995	34.84	0.2800	B,D,F
72	50.21	1.8171	164.62	0.2800	A,B,C,D,E
73	50.38	1.8113	36.54	0.2800	A,C,E
74	53.58	1.7104	29.94	0.2800	C,D,E
75	53.98	1.6986	30.37	0.2800	C,D,E
76	54.31	1.6891	38.56	0.2800	B,C,D,E
77	54.62	1.6802	30.42	0.2800	B,C,D,E
78	54.80	1.6753	42.35	0.2800	A,B,C,D
79	54.97	1.6704	76.75	0.2800	A,B,D
80	55.08	1.6673	33.07	0.2800	C,D
81	55.37	1.6594	57.80	0.2800	A,B,C,D
82	55.67	1.6512	34.71	0.2800	C,D
83	55.83	1.6468	30.38	0.2800	C,D
84	56.17	1.6375	30.41	0.2800	B,C,D,G
85	56.58	1.6266	35.18	0.2800	B,C,D,E,F,G
86	60.02	1.5415	134.41	0.2800	A,C,D,E
87	60.20	1.5372	36.36	0.2800	A,B,C,D,E,F
88	61.91	1.4988	30.15	0.2800	B,C,D,E,G
89	62.10	1.4947	29.04	0.2800	B,C,D
90	62.25	1.4915	50.28	0.2800	B,C,D
91	62.56	1.4848	29.60	0.2800	B,C,D,E
92	64.10	1.4529	29.16	0.2800	A,B,C,D,F,G
93	67.80	1.3822	81.43	0.2800	A,C,D,E
94	68.00	1.3786	38.02	0.2800	A,B,E
95	68.21	1.3750	91.83	0.2800	A,B
96	68.36	1.3723	72.67	0.2800	A,B,C,D,E

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

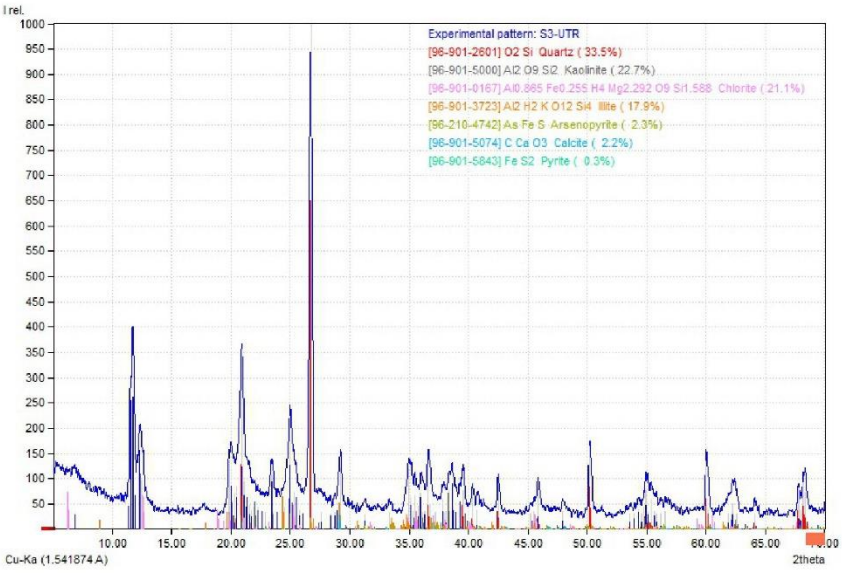
Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	140373	100.00%
Background radiation	76455	54.47%
Diffraction peaks	63918	45.53%
Peak area belonging to selected phases	95362	67.93%
Peak area of phase A (Quartz)	*27204*	*19.38%*
Peak area of phase B (Kaolinite)	*22969*	*16.36%*
Peak area of phase C (Chlorite)	*20830*	*14.84%*
Peak area of phase D (Illite)	*16806*	*11.97%*
Peak area of phase E (Arsenopyrite)	*5077*	*3.62%*
Peak area of phase F (Calcite)	*1955*	*1.39%*
Peak area of phase G (Pyrite)	*522*	*0.37%*
Unidentified peak area	7343	5.23%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	1424	100.00%
Peak intensity belonging to selected phases	-211	-14.87%
Unidentified peak intensity	1635	114.87%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S4-UTR

Sample Data

File name	S4-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S4-UTR
Data collected	Jun 7, 2022 13:00:09
Data range	5.060° - 70.060°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	0.06°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	48.1	Quartz	O2 Si
B	27.7	Pyrite	Cu0.25 Fe0.75 S2
C	10.3	Chalcocite	Cu2 S
D	10.0	Calcite	C Ca O3
E	3.9	Kaolinite	Al2 O9 Si2
	6.3	*Unidentified peak area*	

A: Quartz (48.1 %)

Formula sum	O2 Si
Entry number	96-901-0145
Figure-of-Merit (FoM)	0.819649
Total number of peaks	70
Peaks in range	36
Peaks matched	30
Intensity scale factor	0.38
Space group	P 32 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9230 Å c= 5.4090 Å
I/Ic	2.99
Calc. density	2.636 g/cm³
Reference	Ikuta D., Kawame N., Banno S., Hirajima T., Ito K., Rakovan J. F., Downs R. T., Tamada O., "First in situ X-ray diffraction identification of coesite and retrogradequartz on a glass thin section of an ultrahigh-pressure metamorphic rock andtheir crystal structure details Locality: Yangkou meta-igneous complex in themiddle part of the Sulu UHP terrain, eastern China Note: Sample is on a thinsection", American Mineralogist **92**, 57-63 (2007)

B: Pyrite (27.7 %)

Formula sum	Cu0.25 Fe0.75 S2
Entry number	96-900-6171
Figure-of-Merit (FoM)	0.392101
Total number of peaks	48
Peaks in range	24
Peaks matched	10
Intensity scale factor	0.30
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.7249 Å
I/Ic	4.14
Calc. density	4.315 g/cm³
Reference	Schmid-Beurmann P, Lottermoser W., "57Fe-Moessbauer spectra, electronic and crystal structure of members of theCuS2-FeS2 solid solution series", Physics and Chemistry of Minerals **19**, 571-577 (1993)

C: Chalcocite (10.3 %)

Formula sum	Cu2 S
Entry number	96-900-8288
Figure-of-Merit (FoM)	0.384551
Total number of peaks	994
Peaks in range	994
Peaks matched	281
Intensity scale factor	0.03
Space group	P 1 21/c 1
Crystal system	monoclinic
Unit cell	a= 15.2460 Å b= 11.8840 Å c= 13.4940 Å β= 116.350 °
I/Ic	1.09
Calc. density	5.790 g/cm³
Reference	Evans H. T., "The crystal structures of low chalocite and djurleiteLocality: Bristol Connecticut, USA", Zeitschrift fur Kristallographie **150**, 299-320 (1979)

D: Calcite (10.0 %)

Formula sum	C Ca O3
Entry number	96-901-6465
Figure-of-Merit (FoM)	0.419802
Total number of peaks	86
Peaks in range	36
Peaks matched	6
Intensity scale factor	0.09
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)

Unit cell	a= 4.9775 Å c= 17.2949 Å
I/Ic	3.28
Calc. density	2.685 g/cm³
Reference	Antao S. M., Hassan I., "Temperature dependence of the structural parametersin the transformation of aragonite to calcite,as determined from in situ synchrotron powder X-ray-diffraction dataNote: T = 477 CNote: P = 101 kPa", The Canadian Mineralogist **48**, 1225-1236 (2010)

E: Kaolinite (3.9 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.614341
Total number of peaks	528
Peaks in range	240
Peaks matched	106
Intensity scale factor	0.01
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
	O2 Si	96-710-3015	0.7616
Silicon oxide (Quartz)	O2 Si	96-500-0036	0.7602
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1098	0.7560
Si O2	O2 Si	96-152-6861	0.7541
	O2 Si	96-210-0189	0.7526
Quartz	O2 Si	96-901-3322	0.7526
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1173	0.7524
Quartz	O2 Si	96-901-2601	0.7522
Hg Mn	Hg Mn	96-153-7798	0.7506
Quartz	O2 Si	96-900-9667	0.7465
	O2 Si	96-230-0371	0.7453
hexagonal boron nitride	B N	96-201-6171	0.7427
	B N	96-900-8998	0.7344
Boron Nitride	B N	96-591-0080	0.7339
	O7 P2 Si	96-591-0161	0.7251
	Ge O7 P2	96-591-0254	0.7089
N2 H4 H2 O	H6 N2 O	96-231-0627	0.7073
Si O2	O2 Si	96-153-2513	0.7067
Potassium	K	96-901-1974	0.7051
Ag Mg	Ag Mg	96-150-9457	0.7012
Xenon	Xe	96-901-2406	0.6976
Al P O4	Al O4 P	96-153-0003	0.6962
Li2 Sn Zn	Li2 Sn Zn	96-152-2876	0.6954
Potassium hydrogensulfide - at 473K	H K S	96-101-0905	0.6939
	K S	96-901-4695	0.6939
Uranium trideuteride -$-beta	D3 U	96-100-8630	0.6898
(Eu0.5 Sr0.5) Te	Eu0.5 Sr0.5 Te	96-152-7664	0.6869
Be F2	Be F2	96-153-1932	0.6868
K (N O2)	K N O2	96-810-4318	0.6826
	Al0.05 Li0.05 O2 Si0.95	96-900-2384	0.6826
Ni1.29 Ti3	N1.29 Ti3	96-153-8608	0.6820
	O45 P9 V12	96-400-1392	0.6802
	Ga O4 P	96-151-8035	0.6781
Hg Mn	Hg Mn	96-152-2377	0.6777
Lu Ru	Lu Ru	96-152-3887	0.6772
Iron phosphate hydroxide	Fe1.176 O5 P	96-400-0553	0.6742
Lu Rh	Lu Rh	96-231-0897	0.6741
(Au0.67 Hg0.33) Mg	Au0.67 Hg0.33 Mg	96-151-0379	0.6740
Hydrogen	H2	96-901-3090	0.6680
Si O2	O2 Si	96-153-8065	0.6667
Si (N C S)4	C4 N4 S4 Si	96-154-1742	0.6654
(Ag5 Cd Mg4)0.2	Ag Cd0.2 Mg0.8	96-150-9168	0.6653
O2	O2	96-210-6878	0.6650
Si O2	O2 Si	96-153-6390	0.6637
Uranium trihydride - $-beta	H3 U	96-100-8631	0.6632
Genthelvite	Be3 O12 S Si3 Zn4	96-900-0952	0.6615
	Au Cd	96-900-8804	0.6612
Polonium	Po	96-150-9139	0.6605
Au2 In Sc	Au2 In Sc	96-151-0428	0.6601
Cs2 K Y F6	Cs2 F6 K Y	96-153-9461	0.6600
	Cs2 O8 V3	96-433-4973	0.6591
	Ga O4 P	96-151-8036	0.6585

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number: 96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707;96-101-1046;96-901-5000;96-900-0846;96-900-5551;96-900-8288;96-901-5069

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	6.50	13.6050	14.91	0.2800	
2	6.81	12.9872	16.43	0.2800	
3	7.00	12.6283	13.07	0.2800	
4	11.74	7.5395	14.52	0.2800	
5	12.09	7.3209	31.73	0.2800	
6	12.25	7.2278	38.83	0.2800	
7	12.42	7.1245	43.48	0.2800	E
8	12.54	7.0590	19.35	0.2800	
9	20.02	4.4344	64.96	0.2800	C,E
10	20.16	4.4048	19.48	0.2800	E
11	20.33	4.3682	37.57	0.2800	
12	20.49	4.3353	19.24	0.2800	
13	20.64	4.3032	32.33	0.2800	
14	20.99	4.2325	203.16	0.2800	A,C,E
15	21.37	4.1582	17.13	0.2800	
16	21.51	4.1308	14.50	0.2800	
17	21.72	4.0912	13.09	0.2800	
18	22.07	4.0274	19.90	0.2800	E
19	22.98	3.8705	12.55	0.2800	C,D
20	23.89	3.7244	14.89	0.2800	C
21	24.39	3.6499	14.67	0.2800	
22	24.66	3.6107	20.89	0.2800	C
23	24.98	3.5642	61.92	0.2800	C,E
24	25.10	3.5479	20.42	0.2800	C
25	25.24	3.5286	14.40	0.2800	E
26	25.37	3.5110	25.77	0.2800	C,E
27	26.74	3.3336	1000.00	0.2800	A,B,C
28	27.92	3.1956	15.84	0.2800	C
29	28.09	3.1762	21.59	0.2800	C
30	34.72	2.5841	16.78	0.2800	C,E
31	35.09	2.5571	49.42	0.2800	B,C,E
32	35.28	2.5441	16.19	0.2800	C
33	35.52	2.5276	21.04	0.2800	C,E
34	35.72	2.5140	14.49	0.2800	C
35	35.93	2.4995	24.26	0.2800	
36	36.08	2.4891	18.45	0.2800	C,D,E
37	36.65	2.4519	124.84	0.2800	A,C
38	37.64	2.3895	13.47	0.2800	C,E
39	37.89	2.3744	19.72	0.2800	C,E
40	38.19	2.3568	16.41	0.2800	C
41	38.33	2.3484	17.90	0.2800	C,E
42	38.59	2.3329	36.01	0.2800	B,C
43	38.82	2.3198	15.64	0.2800	C
44	39.04	2.3073	14.95	0.2800	C
45	39.30	2.2923	14.80	0.2800	A,D
46	39.58	2.2772	84.64	0.2800	A,C,D,E
47	40.39	2.2331	44.73	0.2800	A,C,E
48	42.57	2.1237	84.90	0.2800	A,C,E
49	45.34	2.0003	12.42	0.2800	C,E
50	45.93	1.9760	57.92	0.2800	A,C,E
51	50.24	1.8159	162.09	0.2800	A,C
52	54.73	1.6773	14.61	0.2800	A,C,E
53	54.98	1.6702	70.62	0.2800	A,C,E
54	55.30	1.6611	15.62	0.2800	A,C,E
55	55.43	1.6576	22.45	0.2800	A,B,C,E
56	60.04	1.5408	141.46	0.2800	A
57	60.24	1.5363	21.92	0.2800	B,E
58	61.80	1.5013	16.82	0.2800	E
59	62.21	1.4922	26.75	0.2800	E
60	62.38	1.4887	12.51	0.2800	E
61	62.50	1.4860	14.54	0.2800	E
62	64.14	1.4521	27.50	0.2800	A,E
63	67.82	1.3818	67.39	0.2800	A,B
64	68.01	1.3784	18.84	0.2800	A,E
65	68.24	1.3745	75.49	0.2800	A,E
66	68.41	1.3714	61.92	0.2800	A,E

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

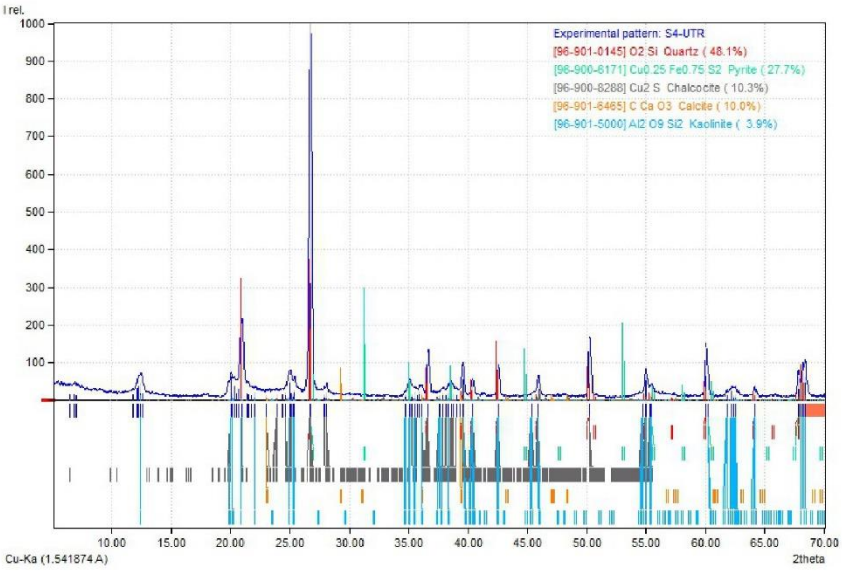
Based on calculated profile

Profile area	*Counts*	*Amount*
Overall diffraction profile	158407	100.00%
Background radiation	78888	49.80%
Diffraction peaks	79519	50.20%
Peak area belonging to selected phases	113750	71.81%
Peak area of phase A (Quartz)	*59768*	*37.73%*
Peak area of phase B (Pyrite)	*18932*	*11.95%*
Peak area of phase C (Chalcocite)	*21322*	*13.46%*
Peak area of phase D (Calcite)	*7022*	*4.43%*
Peak area of phase E (Kaolinite)	*6705*	*4.23%*
Unidentified peak area	9925	6.27%

Peak Residuals

Peak data	*Counts*	*Amount*
Overall peak intensity	1809	100.00%
Peak intensity belonging to selected phases	-162	-9.00%
Unidentified peak intensity	1972	109.00%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S5-UTR

Sample Data

File name	S5-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S5-UTR
Data collected	Jun 7, 2022 13:00:09
Data range	5.030° - 70.030°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	0.03°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	35.9	Illite	Al2 H2 K O12 Si4
B	34.0	Kaolinite	Al2 O9 Si2
C	12.3	Quartz	O2 Si
D	11.4	Chalcocite	Cu2 S
E	3.3	Pyrite	Cu0.6 Fe0.4 S2
F	3.0	Arsenopyrite	As Fe S
	5.9	*Unidentified peak area*	

A: Illite (35.9 %)

Formula sum	Al2 H2 K O12 Si4
Entry number	96-901-3721
Figure-of-Merit (FoM)	0.625582
Total number of peaks	526
Peaks in range	210
Peaks matched	97
Intensity scale factor	0.27
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.2080 Å b= 9.0200 Å c= 10.1660 Å β= 101.500 °
I/Ic	0.89
Calc. density	2.834 g/cm³
Reference	Drits V. A., Zviagina B. B., McCarty D. K., Salyn A. L., "Factors responsible for crystal-chemical variations in the solid solutionsfrom illite to aluminoceladonite and from glauconite to celadoniteLocality: Kaube Mine, Nara Prefecture, JapanSample Name: Silver Hill", American Mineralogist **95**, 348-361 (2010)

B: Kaolinite (34.0 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.735330
Total number of peaks	528
Peaks in range	240
Peaks matched	90
Intensity scale factor	0.33
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

C: Quartz (12.3 %)

Formula sum	O2 Si
Entry number	96-900-9667
Figure-of-Merit (FoM)	0.800152
Total number of peaks	70
Peaks in range	36
Peaks matched	26
Intensity scale factor	0.47
Space group	P 31 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9158 Å c= 5.4091 Å
I/Ic	4.52
Calc. density	2.644 g/cm³
Reference	Gualtieri A. F., "Accuracy of XRPD QPAusing the combined Rietveld-RIR methodLocality: Baveno, Novara, Italy", Journal of Applied Crystallography **33**, 267-278 (2000)

D: Chalcocite (11.4 %)

Formula sum	Cu2 S
Entry number	96-901-5069
Figure-of-Merit (FoM)	0.474672
Total number of peaks	994
Peaks in range	994
Peaks matched	258
Intensity scale factor	0.10
Space group	P 1 21/c 1
Crystal system	monoclinic
Unit cell	a= 15.2460 Å b= 11.8840 Å c= 13.4940 Å β= 116.350 °

I/Ic	1.08
Calc. density	5.790 g/cm³
Reference	Evans H. T., "Crystal structure of low chalcocite", Nature Physical Science **232**, 69-70 (1971)

E: Pyrite (3.3 %)

Formula sum	Cu0.6 Fe0.4 S2
Entry number	96-900-6172
Figure-of-Merit (FoM)	0.567440
Total number of peaks	46
Peaks in range	22
Peaks matched	12
Intensity scale factor	0.11
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.5624 Å
I/Ic	3.91
Calc. density	4.809 g/cm³
Reference	Schmid-Beurmann P, Lottermoser W., "57Fe-Moessbauer spectra, electronic and crystal structure of members of theCuS2-FeS2 solid solution series", Physics and Chemistry of Minerals **19**, 571-577 (1993)

F: Arsenopyrite (3.0 %)

Formula sum	As Fe S
Entry number	96-210-4742
Figure-of-Merit (FoM)	0.460209
Total number of peaks	410
Peaks in range	170
Peaks matched	49
Intensity scale factor	0.06
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 5.7434 Å b= 5.6698 Å c= 5.7871 Å α= 90.000° β= 112.191 ° γ= 90.000 °
I/Ic	2.30
Calc. density	6.198 g/cm³
Reference	Elliot Alexander Dean, "Structure of pyrrhotite 5C (Fe~9~S~10~)", , 1448-1469 (1961)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
Ba45 Cu28 Al17 F197	Al17 Ba45 Cu28 F197	96-153-6586	0.8060
Ni1.29 Ti3	N1.29 Ti3	96-153-8608	0.8025
Cannizzarite	Bi54 Pb46 S127	96-901-1203	0.7949
B2 H6	B2 H6	96-153-5675	0.7884
Antigorite-T	Mg48 O147 Si34	96-901-6234	0.7834
	N	96-151-2523	0.7782
Na (Cl O4)	Cl Na O4	96-722-3700	0.7731
Vandendriesscheite	H33 O48 Pb2 U10	96-900-1892	0.7705
Dickite	Al2 H4 O9 Si2	96-900-0123	0.7680
aluminum phosphate	Al O4 P	96-201-0797	0.7621
Dickite	Al2 H4 O9 Si2	96-900-3082	0.7612
(Pd0.37 Zr0.63)	Pd0.37 Zr0.63	96-152-2585	0.7574
Wakefieldite-(Y)	O2 V Y	96-901-6009	0.7553
	Ag Cl H12 N4 O4	96-433-2266	0.7545
Becquerelite	Ca O30 U6	96-900-1111	0.7533
Li2 (S O4)	Li2 O4 S	96-153-0495	0.7523
Pb0.497 ((U O2)4 O1.994 (O H)5.006) (H2 O)4	H13.006 O19 Pb0.497 U4	96-152-1510	0.7519
Li0.94 Ag2 In1.06	Ag2 In1.06 Li0.94	96-152-8795	0.7511
Richetite	Fe0.47 H24 Mg0.83 O173 Pb8.74 U36	96-900-4468	0.7509
Dickite	Al2 H4 O9 Si2	96-901-3940	0.7491
Ni5 P2	Ni5.09067 P1.998	96-153-8448	0.7476
Si O2	O2 Si	96-412-4034	0.7471
Li Ag2 In	Ag2 In Li	96-150-9647	0.7456
Li (Cl O4)	Cl Li O4	96-153-6553	0.7456
Si O2	O2 Si	96-810-3727	0.7445
I F7	F7 I	96-231-0566	0.7440
	Al O4 P	96-201-2012	0.7436
Dickite	Al2 H4 O9 Si2	96-901-3920	0.7433
Pd Sc	Pd Sc	96-152-3180	0.7431
Becquerelite	Ca H22 O30 U6	96-901-2088	0.7422
	Al O4 P	96-201-2013	0.7412
Fourmarierite	H10 O19 Pb U4	96-900-4592	0.7411
Ce3 Ge5	Ce2.76923 Ge4.30769	96-152-4792	0.7407
Tridymite	O2 Si	96-900-5271	0.7392
Na.5 H2.5 P O3	H2.5 Na0.5 O3 P	96-210-6978	0.7389
(Au0.25 Hg0.75) Mn	Au0.25 Hg0.75 Mn	96-151-0078	0.7354
Villiaumite	F Na	96-900-7463	0.7351
Nb Ta	Nb Ta	96-153-7943	0.7348
	C4 Cl2 F N2 O2 S5	96-411-6447	0.7347
Cristobalite	O2 Si	96-900-8232	0.7345
(Nb Ta)	Nb Ta	96-152-3087	0.7341
Rh Zr	Rh Zr	96-154-0936	0.7340
Niobium	Nb	96-900-8547	0.7339
Hf Tc	Hf Tc	96-152-3440	0.7338
Ta	Ta	96-154-1267	0.7338
	Nb	96-400-0949	0.7336
Villiaumite	F Na	96-900-7464	0.7329
D2 O	D2 O	96-153-8612	0.7327
Villiaumite	F Na	96-900-7462	0.7326
Li2 (S O4)	O4 S	96-153-7067	0.7324
Ice VII	H2 O	96-901-6612	0.7321
Tridymite	O2 Si	96-900-0521	0.7319

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	3
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number: 96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-0846;96-900-5551;96-900-8288;96-901-5069;96-900-1665;96-900-4787;96-900-4919;96-900-7429;96-900-7612;96-900-9523;96-900-9666;96-901-0118;96-901-0494;96-901-0549;96-901-1123;96-901-1745;96-901-1746;96-901-2893;96-901-3719;96-901-3720;96-901-3721;96-901-3722;96-901-3723;96-901-3724;96-901-3733;96-901-3985;96-901-6664;96-101-1046;96-901-5000

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	11.76	7.5272	161.23	0.4000	
2	12.00	7.3778	238.87	0.4000	
3	12.27	7.2137	375.45	0.4000	
4	12.44	7.1182	220.91	0.4000	B
5	12.55	7.0534	123.13	0.4000	
6	19.95	4.4497	623.62	0.4000	A
7	20.12	4.4136	257.11	0.4000	B
8	20.25	4.3854	234.71	0.4000	B
9	20.42	4.3483	300.08	0.4000	A
10	20.62	4.3082	226.83	0.4000	
11	20.83	4.2651	317.06	0.4000	B,C
12	21.03	4.2252	232.77	0.4000	D
13	21.13	4.2047	122.01	0.4000	
14	21.36	4.1602	215.17	0.4000	
15	21.43	4.1459	140.95	0.4000	
16	21.63	4.1080	172.55	0.4000	A
17	21.79	4.0788	132.63	0.4000	
18	22.03	4.0349	164.27	0.4000	B
19	22.24	3.9981	154.08	0.4000	
20	22.50	3.9519	173.16	0.4000	
21	22.73	3.9129	150.43	0.4000	F
22	22.91	3.8819	150.68	0.4000	D,F
23	23.20	3.8337	206.84	0.4000	A,D
24	23.49	3.7880	148.29	0.4000	B,D
25	23.63	3.7650	137.30	0.4000	D
26	23.83	3.7341	138.07	0.4000	D
27	24.05	3.7005	220.87	0.4000	
28	24.25	3.6701	139.69	0.4000	F
29	24.46	3.6392	289.04	0.4000	A,F
30	24.78	3.5936	499.47	0.4000	B,D
31	25.03	3.5579	611.69	0.4000	B,D
32	25.16	3.5392	289.06	0.4000	
33	25.29	3.5217	166.50	0.4000	B
34	25.47	3.4972	275.58	0.4000	
35	25.65	3.4731	157.20	0.4000	
36	25.89	3.4411	238.21	0.4000	D
37	26.29	3.3897	311.31	0.4000	D
38	26.75	3.3328	1000.00	0.4000	A,C,D
39	27.17	3.2816	161.17	0.4000	D
40	27.33	3.2633	134.83	0.4000	B,D
41	27.66	3.2251	211.05	0.4000	E
42	27.90	3.1979	125.15	0.4000	D,E
43	28.15	3.1701	122.50	0.4000	D
44	28.48	3.1336	137.72	0.4000	D
45	28.87	3.0928	147.17	0.4000	
46	29.23	3.0554	107.69	0.4000	A,D
47	29.52	3.0256	103.97	0.4000	B
48	29.81	2.9976	109.27	0.4000	B,D
49	30.11	2.9680	110.76	0.4000	D
50	30.38	2.9421	103.95	0.4000	D
51	30.88	2.8959	98.22	0.4000	A,D,F
52	32.01	2.7963	103.63	0.4000	B,D,E,F
53	34.69	2.5856	200.10	0.4000	A,B,D
54	35.03	2.5616	438.79	0.4000	A,B,D,F
55	35.17	2.5518	171.41	0.4000	A,F
56	35.33	2.5406	128.89	0.4000	B,D,F
57	35.51	2.5280	168.42	0.4000	B,D
58	35.85	2.5046	227.39	0.4000	F
59	36.03	2.4925	178.03	0.4000	A,B,E,F
60	36.33	2.4729	123.47	0.4000	A,B,D
61	36.64	2.4524	198.70	0.4000	A,C,D,F
62	37.23	2.4151	137.45	0.4000	B,D,F
63	37.53	2.3964	159.32	0.4000	A,B,D,F

64	37.75	2.3833	132.63	0.4000	B,D,F
65	37.86	2.3762	129.15	0.4000	D
66	38.04	2.3654	177.23	0.4000	A,D
67	38.37	2.3459	309.55	0.4000	A,B,D
68	38.57	2.3342	235.49	0.4000	D
69	38.84	2.3185	236.53	0.4000	D
70	39.34	2.2906	187.62	0.4000	C
71	40.30	2.2382	143.64	0.4000	A,B,C,D
72	42.62	2.1216	107.05	0.4000	A,B,C,D
73	45.75	1.9833	98.83	0.4000	A,B,C,D
74	50.23	1.8164	125.13	0.4000	A,C,D,F
75	54.31	1.6892	136.80	0.4000	A,B,D,F
76	54.63	1.6801	129.40	0.4000	B,D,E,F
77	54.83	1.6745	100.60	0.4000	A,B,C,D,E
78	55.02	1.6690	117.50	0.4000	A,B,C,D
79	55.23	1.6632	134.38	0.4000	A,B,C,D
80	55.46	1.6570	126.80	0.4000	A,B,C,D
81	55.71	1.6501	148.83	0.4000	A
82	56.39	1.6317	111.39	0.4000	A,B,F
83	60.05	1.5407	125.72	0.4000	A,B,C,E,F
84	61.87	1.4997	129.69	0.4000	A,B,F
85	62.24	1.4917	234.28	0.4000	A
86	62.35	1.4892	96.70	0.4000	A,B,E
87	62.53	1.4853	97.01	0.4000	A,B,E,F
88	68.23	1.3746	120.17	0.4000	A,B,C,F

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

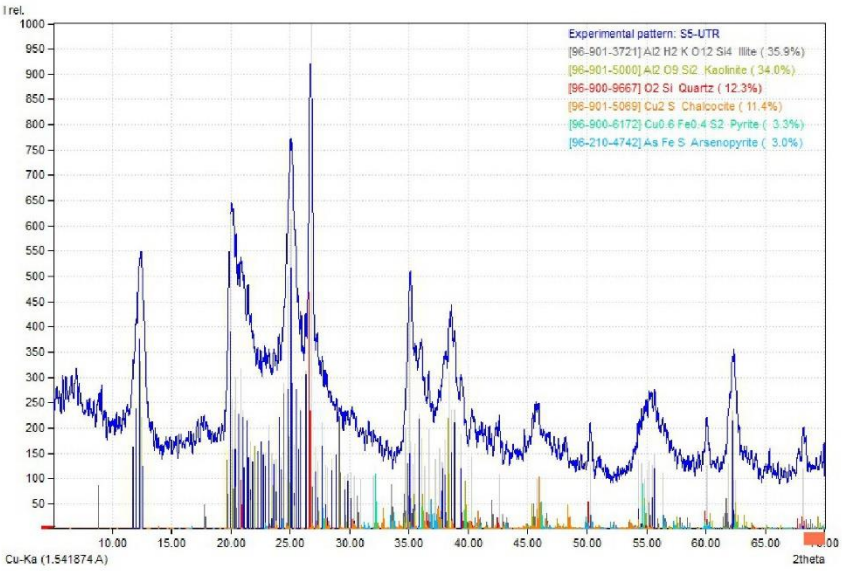
Based on calculated profile

Profile area	*Counts*	*Amount*
Overall diffraction profile	182429	100.00%
Background radiation	110437	60.54%
Diffraction peaks	71992	39.46%
Peak area belonging to selected phases	101387	55.58%
Peak area of phase A (Illite)	*30203*	*16.56%*
Peak area of phase B (Kaolinite)	*30408*	*16.67%*
Peak area of phase C (Quartz)	*10223*	*5.60%*
Peak area of phase D (Chalcocite)	*19735*	*10.82%*
Peak area of phase E (Pyrite)	*4867*	*2.67%*
Peak area of phase F (Arsenopyrite)	*5951*	*3.26%*
Unidentified peak area	10708	5.87%

Peak Residuals

Peak data	*Counts*	*Amount*
Overall peak intensity	1684	100.00%
Peak intensity belonging to selected phases	-19	-1.20%
Unidentified peak intensity	1704	101.20%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S6-UTR

Sample Data

File name	S6-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S6-UTR
Data collected	Jun 7, 2022 13:00:10
Data range	4.950° - 69.950°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	No
2theta correction	-0.05°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	66.4	Quartz	O2 Si
B	14.0	Chlorite	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
C	7.6	Barite	Ba O4 S
D	5.7	Biotite	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
E	5.6	Gypsum	Ca H4 O6 S
F	0.7	Pyrite	Fe S2
	7.0	*Unidentified peak area*	

A: Quartz (66.4 %)

Formula sum	O2 Si
Entry number	96-900-5018
Figure-of-Merit (FoM)	0.885992
Total number of peaks	70
Peaks in range	36
Peaks matched	31
Intensity scale factor	0.38
Space group	P 32 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9137 Å c= 5.4047 Å
I/Ic	2.99
Calc. density	2.649 g/cm³
Reference	Kihara K., "An X-ray study of the temperature dependence of the quartz structureSample: at T = 298 K", European Journal of Mineralogy **2**, 63-77 (1990)

B: Chlorite (14.0 %)

Formula sum	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
Entry number	96-901-0164
Figure-of-Merit (FoM)	0.390691
Total number of peaks	600
Peaks in range	311
Peaks matched	109
Intensity scale factor	0.02
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.3363 Å b= 9.2400 Å c= 14.3700 Å β= 96.930 °
I/Ic	0.81
Calc. density	2.700 g/cm³
Reference	Zanazzi P. F., Montagnoli M., Nazzareni S., Comodi P., "Structural effects of pressure on monoclinic chlorite: a single-crystal studyLocality: Alpe Raguzzolo, Val Malenco, Italy Sample: P = 0.0001 GPa", American Mineralogist **92**, 655-661 (2007)

C: Barite (7.6 %)

Formula sum	Ba O4 S
Entry number	96-900-0160
Figure-of-Merit (FoM)	0.404140
Total number of peaks	404
Peaks in range	175
Peaks matched	63
Intensity scale factor	0.05
Space group	P n m a
Crystal system	orthorhombic
Unit cell	a= 8.8840 Å b= 5.4580 Å c= 7.1530 Å
I/Ic	3.21
Calc. density	4.469 g/cm³
Reference	Colville A. A., Staudhammer K., "Arefinement of the structure of baritefrom Cow Green mine", American Mineralogist **52**, 1877-1880 (1967)

D: Biotite (5.7 %)

Formula sum	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
Entry number	96-900-1583
Figure-of-Merit (FoM)	0.686993
Total number of peaks	548
Peaks in range	220
Peaks matched	67
Intensity scale factor	0.05
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.3350 Å b= 9.2440 Å c= 10.2060 Å β= 100.080 °

I/Ic	4.72
Calc. density	2.794 g/cm³
Reference	Bigi S., Brigatti M. F., "Crystal chemistry and microstructures of plutonic biotiteSample 1M from Valle del Cervo syenitic complex", American Mineralogist **79**, 63-72 (1994)

E: Gypsum (5.6 %)

Formula sum	Ca H4 O6 S
Entry number	96-901-3171
Figure-of-Merit (FoM)	0.497080
Total number of peaks	478
Peaks in range	200
Peaks matched	57
Intensity scale factor	0.02
Space group	C 1 2/c 1
Crystal system	monoclinic
Unit cell	a= 6.1620 Å b= 14.9650 Å c= 5.5800 Å β= 115.380 °
I/Ic	2.01
Calc. density	2.459 g/cm³
Reference	Comodi P., Nazzareni S., Zanazzi P. F., Speziale S., "High-pressure behavior of gypsum: A single-crystal X-ray studyLocality: Valle di Caramanico, Abruzzo, ItalyNote: P = 3.15 GPa", American Mineralogist **93**, 1530-1537 (2008)

F: Pyrite (0.7 %)

Formula sum	Fe S2
Entry number	96-900-0595
Figure-of-Merit (FoM)	0.158017
Total number of peaks	42
Peaks in range	20
Peaks matched	7
Intensity scale factor	0.00
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.4166 Å
I/Ic	3.34
Calc. density	5.014 g/cm³
Reference	Bayliss P., "Crystal structure refinement of a weakly anisotropic pyritecubic model", American Mineralogist **62**, 1168-1172 (1977)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
	Al9 Ni3 Y	96-210-0949	0.7045
	B17 Be N2	96-210-1329	0.6998
	O2 Si	96-710-3015	0.6895
	Fe0.91 Si0.09	96-900-6615	0.6874
Silicon oxide (Quartz)	O2 Si	96-500-0036	0.6866
Quartz	O2 Si	96-901-2601	0.6848
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1173	0.6846
	B N	96-900-8998	0.6844
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1098	0.6843
	O2 Si	96-210-0189	0.6843
Quartz	O2 Si	96-901-3322	0.6841
Boron Nitride	B N	96-591-0080	0.6787
	Al9 Dy Ni3	96-210-0950	0.6781
Si O2	O2 Si	96-412-4034	0.6753
Quartz	O2 Si	96-900-9667	0.6742
	O2 Si	96-230-0371	0.6720
	Ge O7 P2	96-591-0254	0.6684
	O7 P2 Si	96-591-0161	0.6665
hexagonal boron nitride	B N	96-201-6171	0.6664
Si O2	O2 Si	96-153-2513	0.6653
	Al0.05 Li0.05 O2 Si0.95	96-900-2384	0.6542
Si O2	O2 Si	96-152-6861	0.6523
	Al9 Gd Ni3	96-210-0948	0.6463
Potassium	K	96-901-1974	0.6449
(Ru (C O)3)4 Se4	C12 O12 Ru4 Se4	96-403-1214	0.6424
Be F2	Be F2	96-153-1932	0.6369
N2 H4 H2 O	H6 N2 O	96-231-0627	0.6357
Ta6 Cl15	Cl15 Ta6	96-153-4241	0.6354
(Nb Ta)	Nb Ta	96-152-3087	0.6343
Na0.364 Mn O2 (H2 O)0.544	H1.088 Mn Na0.364 O2.544	96-153-1680	0.6339
Ta	Ta	96-154-1267	0.6338
Tantalum	Ta	96-900-8553	0.6333
Villiaumite	F Na	96-900-7463	0.6303
	Ta	96-151-2545	0.6291
Villiaumite	F Na	96-900-7464	0.6285
Al P O4	Al O4 P	96-153-0003	0.6282
Pt Zr	Pt Zr	96-152-3370	0.6277
Li Ag1.86 In1.14	Ag1.86 In1.14 Li	96-150-9615	0.6258
	F15 Mo5 O15 Rb15	96-450-8553	0.6249
	H0.9 Na0.22 O2.45 Ru	96-431-0643	0.6242
Au Sn Tm	Au Sn Tm	96-151-0304	0.6221
Fe2 Mn Si	Fe2 Mn Si	96-153-9792	0.6220
	Nb Te4	96-210-1238	0.6202
Berlinite	Al O4 P	96-901-0368	0.6198
Ice VII	H2 O	96-901-6612	0.6189
	Ag2 Li Sn	96-720-4712	0.6183
(Ag5 Cd Mg4)0.2	Ag Cd0.2 Mg0.8	96-150-9168	0.6165
(Ni0.77 Ta0.23)	Ni0.77 Ta0.23	96-152-2811	0.6154
Ag Mg	Ag Mg	96-150-9457	0.6149
Pt Sn U	Pt Sn U	96-152-2662	0.6149
	Fe0.91 Si0.09	96-900-6619	0.6132
Au Er Sn	Au Er Sn	96-151-0130	0.6128

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number:

96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-1226;96-900-1227;96-900-1228;96-900-1245;96-900-4374;96-900-4375;96-900-4376;96-900-4377;96-900-4378;96-900-4379;96-900-4380;96-900-4381;96-900-4384;96-900-4434;96-900-5257;96-900-9977;96-100-0039;96-900-0026;96-900-0468;96-900-0469;96-900-0744;96-900-0843;96-900-0844;96-900-0845;96-900-1265;96-900-1266;96-900-1267;96-900-1268;96-900-1269;96-900-1347;96-900-1348;96-900-1349;96-900-1350;96-900-1351;96-900-1352;96-900-1353;96-900-1354;96-900-1583;96-900-1584;96-900-2302;96-900-2303;96-900-2304;96-900-2305;96-900-2306;96-900-2307;96-900-2308;96-224-1551;96-900-0846;96-900-1182;96-900-1183;96-900-1491;96-900-3581;96-900-4989;96-900-5551;96-900-8012;96-900-8288;96-900-8291;96-900-9255;96-900-9360;96-900-9504;96-900-9831;96-901-4624;96-901-5069;96-901-5557;96-201-4618;96-201-4619;96-201-4931;96-220-5377;96-220-7380;96-220-7381;96-901-0164;96-901-0165;96-901-0166;96-901-0167;96-901-0168;96-901-0169;96-901-0170;96-100-0038;96-500-0046;96-900-0160;96-900-0651;96-900-4123;96-900-4486;96-901-1344;96-901-1419;96-901-4890;96-101-0982;96-101-1075;96-230-0259;96-500-0040;96-900-1752;96-900-1753;96-900-1754;96-900-6647;96-901-3165;96-901-3166;96-901-3167;96-901-3168;96-901-3169;96-901-3170;96-901-3171;96-901-3172;96-901-5351

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	6.81	12.9802	9.33	0.2000	
2	8.80	10.0465	11.14	0.2000	D
3	11.95	7.4061	16.00	0.2000	E
4	12.33	7.1806	177.76	0.2000	
5	12.41	7.1326	58.15	0.2000	B
6	13.86	6.3892	11.62	0.2000	
7	19.76	4.4930	15.16	0.2000	B,D
8	19.88	4.4655	16.59	0.2000	
9	20.01	4.4373	14.56	0.2000	C
10	20.13	4.4113	8.90	0.2000	B,D
11	20.26	4.3842	15.94	0.2000	B
12	20.36	4.3623	17.51	0.2000	
13	20.47	4.3388	15.04	0.2000	C
14	20.91	4.2490	221.17	0.2000	A,B
15	21.21	4.1890	30.36	0.2000	D,E
16	21.35	4.1617	21.41	0.2000	E
17	21.53	4.1275	15.31	0.2000	
18	22.02	4.0369	9.18	0.2000	B
19	23.05	3.8579	13.27	0.2000	B,C
20	23.16	3.8405	9.33	0.2000	
21	23.57	3.7755	17.36	0.2000	C
22	23.71	3.7531	10.10	0.2000	E
23	24.45	3.6405	10.62	0.2000	D
24	24.92	3.5728	166.68	0.2000	B,C
25	25.72	3.4635	14.32	0.2000	B,C
26	26.23	3.3976	10.26	0.2000	D
27	26.68	3.3411	1000.00	0.2000	A,B,C,D
28	27.52	3.2413	39.61	0.2000	
29	27.93	3.1941	74.25	0.2000	
30	29.91	2.9876	13.00	0.2000	B,E
31	34.51	2.5988	10.27	0.2000	E
32	34.70	2.5853	10.45	0.2000	B
33	34.99	2.5642	25.59	0.2000	E
34	35.14	2.5538	10.48	0.2000	B,E
35	35.43	2.5337	12.68	0.2000	B
36	35.60	2.5216	10.85	0.2000	D,E
37	35.93	2.4993	17.87	0.2000	D,E
38	36.19	2.4821	9.86	0.2000	C,E
39	36.58	2.4563	97.29	0.2000	A,B,C,D,E
40	37.76	2.3827	21.91	0.2000	B,E
41	38.45	2.3414	23.48	0.2000	
42	38.57	2.3343	11.73	0.2000	C
43	39.51	2.2810	67.44	0.2000	A,B,C,D
44	40.33	2.2365	40.62	0.2000	A,B,C,D,E
45	41.74	2.1641	13.03	0.2000	B,C,D,E
46	42.49	2.1277	75.86	0.2000	A
47	42.59	2.1228	9.11	0.2000	A,B,C
48	45.40	1.9977	13.42	0.2000	B,D,E
49	45.55	1.9916	10.92	0.2000	B,D,E
50	45.82	1.9802	51.47	0.2000	A,B,E
51	45.95	1.9751	12.01	0.2000	A,D,E
52	50.17	1.8185	137.56	0.2000	A,B,E
53	50.33	1.8130	28.47	0.2000	A,E,F
54	51.12	1.7867	10.14	0.2000	B,C

55	54.91	1.6722	55.64	0.2000	A,B,C,D
56	55.03	1.6688	17.28	0.2000	A,B,C
57	55.33	1.6606	25.03	0.2000	A,B,C,E
58	55.43	1.6577	10.43	0.2000	A,B,C,E
59	55.57	1.6539	9.19	0.2000	B,D
60	56.56	1.6271	8.59	0.2000	C,D,F
61	56.82	1.6205	8.60	0.2000	B,C,D
62	59.74	1.5480	8.89	0.2000	B,D,E
63	59.97	1.5426	111.18	0.2000	A,B,D
64	60.13	1.5389	37.13	0.2000	A,B,C,D,E
65	61.70	1.5034	9.00	0.2000	B,E,F
66	62.13	1.4941	10.23	0.2000	B,C,E
67	62.32	1.4899	14.77	0.2000	B,E
68	64.03	1.4541	13.20	0.2000	A,B,C
69	64.22	1.4503	8.68	0.2000	A,B,C,E,F
70	67.76	1.3830	59.93	0.2000	A,B,C,E
71	67.98	1.3790	31.71	0.2000	A,B,C
72	68.16	1.3758	71.27	0.2000	A,B,C
73	68.32	1.3730	60.70	0.2000	A,B,C,E
74	68.53	1.3693	17.37	0.2000	A,B,C,D,E

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

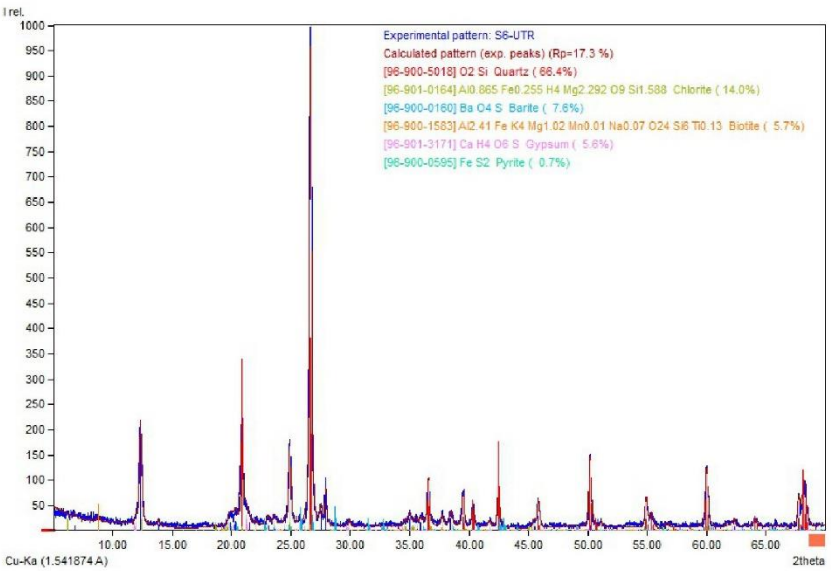
Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	153906	100.00%
Background radiation	64152	41.68%
Diffraction peaks	89754	58.32%
Peak area belonging to selected phases	116069	75.42%
Peak area of phase A (Quartz)	*61244*	*39.79%*
Peak area of phase B (Chlorite)	*18363*	*11.93%*
Peak area of phase C (Barite)	*20236*	*13.15%*
Peak area of phase D (Biotite)	*7690*	*5.00%*
Peak area of phase E (Gypsum)	*7219*	*4.69%*
Peak area of phase F (Pyrite)	*1316*	*0.85%*
Unidentified peak area	10849	7.05%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	1568	100.00%
Peak intensity belonging to selected phases	225	14.37%
Unidentified peak intensity	1343	85.63%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S6-UTR

Sample Data

File name	S6-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S6-UTR
Data collected	Jun 7, 2022 13:00:10
Data range	4.950° - 69.950°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	No
2theta correction	-0.05°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	66.4	Quartz	O2 Si
B	14.0	Chlorite	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
C	7.6	Barite	Ba O4 S
D	5.7	Biotite	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
E	5.6	Gypsum	Ca H4 O6 S
F	0.7	Pyrite	Fe S2
	7.0	*Unidentified peak area*	

A: Quartz (66.4 %)

Formula sum	O2 Si
Entry number	96-900-5018
Figure-of-Merit (FoM)	0.885992
Total number of peaks	70
Peaks in range	36
Peaks matched	31
Intensity scale factor	0.38
Space group	P 32 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9137 Å c= 5.4047 Å
I/Ic	2.99
Calc. density	2.649 g/cm³
Reference	Kihara K., "An X-ray study of the temperature dependence of the quartz structureSample: at T = 298 K", European Journal of Mineralogy **2**, 63-77 (1990)

B: Chlorite (14.0 %)

Formula sum	Al0.865 Fe0.255 H4 Mg2.292 O9 Si1.588
Entry number	96-901-0164
Figure-of-Merit (FoM)	0.390691
Total number of peaks	600
Peaks in range	311
Peaks matched	109
Intensity scale factor	0.02
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.3363 Å b= 9.2400 Å c= 14.3700 Å β= 96.930 °
I/Ic	0.81
Calc. density	2.700 g/cm³
Reference	Zanazzi P. F., Montagnoli M., Nazzareni S., Comodi P., "Structural effects of pressure on monoclinic chlorite: a single-crystal studyLocality: Alpe Raguzzolo, Val Malenco, Italy Sample: P = 0.0001 GPa", American Mineralogist **92**, 655-661 (2007)

C: Barite (7.6 %)

Formula sum	Ba O4 S
Entry number	96-900-0160
Figure-of-Merit (FoM)	0.404140
Total number of peaks	404
Peaks in range	175
Peaks matched	63
Intensity scale factor	0.05
Space group	P n m a
Crystal system	orthorhombic
Unit cell	a= 8.8840 Å b= 5.4580 Å c= 7.1530 Å
I/Ic	3.21
Calc. density	4.469 g/cm³
Reference	Colville A. A., Staudhammer K., "Arefinement of the structure of baritefrom Cow Green mine", American Mineralogist **52**, 1877-1880 (1967)

D: Biotite (5.7 %)

Formula sum	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
Entry number	96-900-1583
Figure-of-Merit (FoM)	0.686993
Total number of peaks	548
Peaks in range	220
Peaks matched	67
Intensity scale factor	0.05
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.3350 Å b= 9.2440 Å c= 10.2060 Å β= 100.080 °

I/Ic	4.72
Calc. density	2.794 g/cm³
Reference	Bigi S., Brigatti M. F., "Crystal chemistry and microstructures of plutonic biotiteSample 1M from Valle del Cervo syenitic complex", American Mineralogist **79**, 63-72 (1994)

E: Gypsum (5.6 %)

Formula sum	Ca H4 O6 S
Entry number	96-901-3171
Figure-of-Merit (FoM)	0.497080
Total number of peaks	478
Peaks in range	200
Peaks matched	57
Intensity scale factor	0.02
Space group	C 1 2/c 1
Crystal system	monoclinic
Unit cell	a= 6.1620 Å b= 14.9650 Å c= 5.5800 Å β= 115.380 °
I/Ic	2.01
Calc. density	2.459 g/cm³
Reference	Comodi P., Nazzareni S., Zanazzi P. F., Speziale S., "High-pressure behavior of gypsum: A single-crystal X-ray studyLocality: Valle di Caramanico, Abruzzo, ItalyNote: P = 3.15 GPa", American Mineralogist **93**, 1530-1537 (2008)

F: Pyrite (0.7 %)

Formula sum	Fe S2
Entry number	96-900-0595
Figure-of-Merit (FoM)	0.158017
Total number of peaks	42
Peaks in range	20
Peaks matched	7
Intensity scale factor	0.00
Space group	P a -3
Crystal system	cubic
Unit cell	a= 5.4166 Å
I/Ic	3.34
Calc. density	5.014 g/cm³
Reference	Bayliss P., "Crystal structure refinement of a weakly anisotropic pyritecubic model", American Mineralogist **62**, 1168-1172 (1977)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
	Al9 Ni3 Y	96-210-0949	0.7045
	B17 Be N2	96-210-1329	0.6998
	O2 Si	96-710-3015	0.6895
	Fe0.91 Si0.09	96-900-6615	0.6874
Silicon oxide (Quartz)	O2 Si	96-500-0036	0.6866
Quartz	O2 Si	96-901-2601	0.6848
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1173	0.6846
	B N	96-900-8998	0.6844
Silicon oxide $-alpha (Quartz low)	O2 Si	96-101-1098	0.6843
	O2 Si	96-210-0189	0.6843
Quartz	O2 Si	96-901-3322	0.6841
Boron Nitride	B N	96-591-0080	0.6787
	Al9 Dy Ni3	96-210-0950	0.6781
Si O2	O2 Si	96-412-4034	0.6753
Quartz	O2 Si	96-900-9667	0.6742
	O2 Si	96-230-0371	0.6720
	Ge O7 P2	96-591-0254	0.6684
	O7 P2 Si	96-591-0161	0.6665
hexagonal boron nitride	B N	96-201-6171	0.6664
Si O2	O2 Si	96-153-2513	0.6653
	Al0.05 Li0.05 O2 Si0.95	96-900-2384	0.6542
Si O2	O2 Si	96-152-6861	0.6523
	Al9 Gd Ni3	96-210-0948	0.6463
Potassium	K	96-901-1974	0.6449
(Ru (C O)3)4 Se4	C12 O12 Ru4 Se4	96-403-1214	0.6424
Be F2	Be F2	96-153-1932	0.6369
N2 H4 H2 O	H6 N2 O	96-231-0627	0.6357
Ta6 Cl15	Cl15 Ta6	96-153-4241	0.6354
(Nb Ta)	Nb Ta	96-152-3087	0.6343
Na0.364 Mn O2 (H2 O)0.544	H1.088 Mn Na0.364 O2.544	96-153-1680	0.6339
Ta	Ta	96-154-1267	0.6338
Tantalum	Ta	96-900-8553	0.6333
Villiaumite	F Na	96-900-7463	0.6303
	Ta	96-151-2545	0.6291
Villiaumite	F Na	96-900-7464	0.6285
Al P O4	Al O4 P	96-153-0003	0.6282
Pt Zr	Pt Zr	96-152-3370	0.6277
Li Ag1.86 In1.14	Ag1.86 In1.14 Li	96-150-9615	0.6258
	F15 Mo5 O15 Rb15	96-450-8553	0.6249
	H0.9 Na0.22 O2.45 Ru	96-431-0643	0.6242
Au Sn Tm	Au Sn Tm	96-151-0304	0.6221
Fe2 Mn Si	Fe2 Mn Si	96-153-9792	0.6220
	Nb Te4	96-210-1238	0.6202
Berlinite	Al O4 P	96-901-0368	0.6198
Ice VII	H2 O	96-901-6612	0.6189
	Ag2 Li Sn	96-720-4712	0.6183
(Ag5 Cd Mg4)0.2	Ag Cd0.2 Mg0.8	96-150-9168	0.6165
(Ni0.77 Ta0.23)	Ni0.77 Ta0.23	96-152-2811	0.6154
Ag Mg	Ag Mg	96-150-9457	0.6149
Pt Sn U	Pt Sn U	96-152-2662	0.6149
	Fe0.91 Si0.09	96-900-6619	0.6132
Au Er Sn	Au Er Sn	96-151-0130	0.6128

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number:

96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-1226;96-900-1227;96-900-1228;96-900-1245;96-900-4374;96-900-4375;96-900-4376;96-900-4377;96-900-4378;96-900-4379;96-900-4380;96-900-4381;96-900-4384;96-900-4434;96-900-5257;96-900-9977;96-100-0039;96-900-0026;96-900-0468;96-900-0469;96-900-0744;96-900-0843;96-900-0844;96-900-0845;96-900-1265;96-900-1266;96-900-1267;96-900-1268;96-900-1269;96-900-1347;96-900-1348;96-900-1349;96-900-1350;96-900-1351;96-900-1352;96-900-1353;96-900-1354;96-900-1583;96-900-1584;96-900-2302;96-900-2303;96-900-2304;96-900-2305;96-900-2306;96-900-2307;96-900-2308;96-224-1551;96-900-0846;96-900-1182;96-900-1183;96-900-1491;96-900-3581;96-900-4989;96-900-5551;96-900-8012;96-900-8288;96-900-8291;96-900-9255;96-900-9360;96-900-9504;96-900-9831;96-901-4624;96-901-5069;96-901-5557;96-201-4618;96-201-4619;96-201-4931;96-220-5377;96-220-7380;96-220-7381;96-901-0164;96-901-0165;96-901-0166;96-901-0167;96-901-0168;96-901-0169;96-901-0170;96-100-0038;96-500-0046;96-900-0160;96-900-0651;96-900-4123;96-900-4486;96-901-1344;96-901-1419;96-901-4890;96-101-0982;96-101-1075;96-230-0259;96-500-0040;96-900-1752;96-900-1753;96-900-1754;96-900-6647;96-901-3165;96-901-3166;96-901-3167;96-901-3168;96-901-3169;96-901-3170;96-901-3171;96-901-3172;96-901-5351

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	6.81	12.9802	9.33	0.2000	
2	8.80	10.0465	11.14	0.2000	D
3	11.95	7.4061	16.00	0.2000	E
4	12.33	7.1806	177.76	0.2000	
5	12.41	7.1326	58.15	0.2000	B
6	13.86	6.3892	11.62	0.2000	
7	19.76	4.4930	15.16	0.2000	B,D
8	19.88	4.4655	16.59	0.2000	
9	20.01	4.4373	14.56	0.2000	C
10	20.13	4.4113	8.90	0.2000	B,D
11	20.26	4.3842	15.94	0.2000	B
12	20.36	4.3623	17.51	0.2000	
13	20.47	4.3388	15.04	0.2000	C
14	20.91	4.2490	221.17	0.2000	A,B
15	21.21	4.1890	30.36	0.2000	D,E
16	21.35	4.1617	21.41	0.2000	E
17	21.53	4.1275	15.31	0.2000	
18	22.02	4.0369	9.18	0.2000	B
19	23.05	3.8579	13.27	0.2000	B,C
20	23.16	3.8405	9.33	0.2000	
21	23.57	3.7755	17.36	0.2000	C
22	23.71	3.7531	10.10	0.2000	E
23	24.45	3.6405	10.62	0.2000	D
24	24.92	3.5728	166.68	0.2000	B,C
25	25.72	3.4635	14.32	0.2000	B,C
26	26.23	3.3976	10.26	0.2000	D
27	26.68	3.3411	1000.00	0.2000	A,B,C,D
28	27.52	3.2413	39.61	0.2000	
29	27.93	3.1941	74.25	0.2000	
30	29.91	2.9876	13.00	0.2000	B,E
31	34.51	2.5988	10.27	0.2000	E
32	34.70	2.5853	10.45	0.2000	B
33	34.99	2.5642	25.59	0.2000	E
34	35.14	2.5538	10.48	0.2000	B,E
35	35.43	2.5337	12.68	0.2000	B
36	35.60	2.5216	10.85	0.2000	D,E
37	35.93	2.4993	17.87	0.2000	D,E
38	36.19	2.4821	9.86	0.2000	C,E
39	36.58	2.4563	97.29	0.2000	A,B,C,D,E
40	37.76	2.3827	21.91	0.2000	B,E
41	38.45	2.3414	23.48	0.2000	
42	38.57	2.3343	11.73	0.2000	C
43	39.51	2.2810	67.44	0.2000	A,B,C,D
44	40.33	2.2365	40.62	0.2000	A,B,C,D,E
45	41.74	2.1641	13.03	0.2000	B,C,D,E
46	42.49	2.1277	75.86	0.2000	A
47	42.59	2.1228	9.11	0.2000	A,B,C
48	45.40	1.9977	13.42	0.2000	B,D,E
49	45.55	1.9916	10.92	0.2000	B,D,E
50	45.82	1.9802	51.47	0.2000	A,B,E
51	45.95	1.9751	12.01	0.2000	A,D,E
52	50.17	1.8185	137.56	0.2000	A,B,E
53	50.33	1.8130	28.47	0.2000	A,E,F
54	51.12	1.7867	10.14	0.2000	B,C

55	54.91	1.6722	55.64	0.2000	A,B,C,D
56	55.03	1.6688	17.28	0.2000	A,B,C
57	55.33	1.6606	25.03	0.2000	A,B,C,E
58	55.43	1.6577	10.43	0.2000	A,B,C,E
59	55.57	1.6539	9.19	0.2000	B,D
60	56.56	1.6271	8.59	0.2000	C,D,F
61	56.82	1.6205	8.60	0.2000	B,C,D
62	59.74	1.5480	8.89	0.2000	B,D,E
63	59.97	1.5426	111.18	0.2000	A,B,D
64	60.13	1.5389	37.13	0.2000	A,B,C,D,E
65	61.70	1.5034	9.00	0.2000	B,E,F
66	62.13	1.4941	10.23	0.2000	B,C,E
67	62.32	1.4899	14.77	0.2000	B,E
68	64.03	1.4541	13.20	0.2000	A,B,C
69	64.22	1.4503	8.68	0.2000	A,B,C,E,F
70	67.76	1.3830	59.93	0.2000	A,B,C,E
71	67.98	1.3790	31.71	0.2000	A,B,C
72	68.16	1.3758	71.27	0.2000	A,B,C
73	68.32	1.3730	60.70	0.2000	A,B,C,E
74	68.53	1.3693	17.37	0.2000	A,B,C,D,E

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

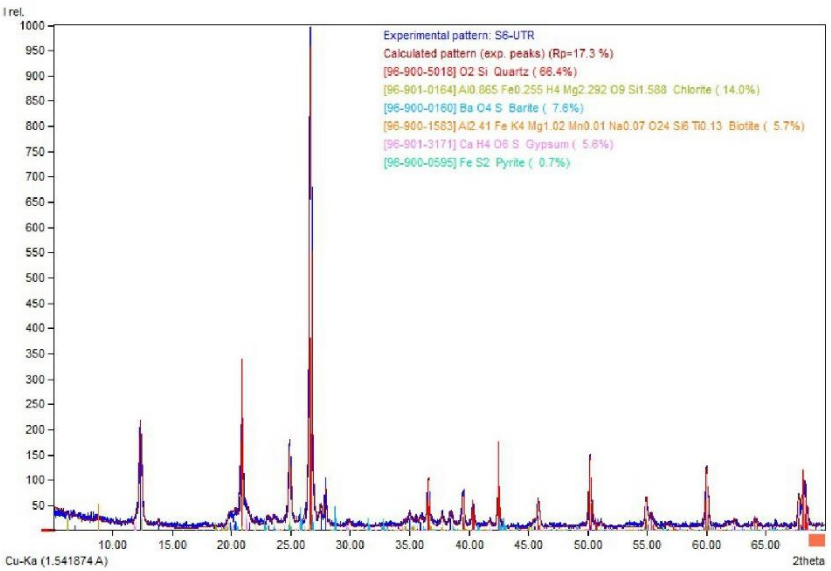
Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	153906	100.00%
Background radiation	64152	41.68%
Diffraction peaks	89754	58.32%
Peak area belonging to selected phases	116069	75.42%
Peak area of phase A (Quartz)	*61244*	*39.79%*
Peak area of phase B (Chlorite)	*18363*	*11.93%*
Peak area of phase C (Barite)	*20236*	*13.15%*
Peak area of phase D (Biotite)	*7690*	*5.00%*
Peak area of phase E (Gypsum)	*7219*	*4.69%*
Peak area of phase F (Pyrite)	*1316*	*0.85%*
Unidentified peak area	10849	7.05%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	1568	100.00%
Peak intensity belonging to selected phases	225	14.37%
Unidentified peak intensity	1343	85.63%

Diffraction Pattern Graphics



Match! Phase Analysis Report

Sample: S7-UTR

Sample Data

File name	S7-UTR.txt
File path	D:/KAMPUS/S2 UNHAS/TESIS/PENGUJIAN LAB/XRD/Analisis/S7-UTR
Data collected	Jun 7, 2022 13:00:10
Data range	4.990° - 69.990°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	-0.01°
Radiation	X-rays
Wavelength	1.541874 Å

Matched Phases

Index	*Amount (%)*	*Name*	*Formula sum*
A	62.3	Quartz	O2 Si
B	14.3	Kaolinite	Al2 O9 Si2
C	8.5	Hornblende	Al5 Ca4 Fe4 H4 Mg4.37 Na1.33 O48 Si13 Ti0.14
D	8.5	Illite	Al2 H2 K O12 Si4
E	3.3	Pyrite	Fe S2
F	3.1	Biotite	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
	1.2	*Unidentified peak area*	

A: Quartz (62.3 %)

Formula sum	O2 Si
Entry number	96-901-3322
Figure-of-Merit (FoM)	0.891510
Total number of peaks	70
Peaks in range	36
Peaks matched	31
Intensity scale factor	0.65
Space group	P 32 2 1
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9134 Å c= 5.4051 Å
I/Ic	4.73
Calc. density	2.649 g/cm³
Reference	Antao S. M., Hassan I., Wang J., Lee P. L., Toby B. H., "State-of-the-art high-resolution powder x-ray diffraction (HRPXRD)illustrated with Rietveld structure refinement of quartz, sodalite,tremolite, and meionite Locality: not specified", The Canadian Mineralogist **46**, 1501-1509 (2008)

B: Kaolinite (14.3 %)

Formula sum	Al2 O9 Si2
Entry number	96-901-5000
Figure-of-Merit (FoM)	0.642984
Total number of peaks	528
Peaks in range	240
Peaks matched	107
Intensity scale factor	0.04
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/Ic	1.16
Calc. density	2.568 g/cm³
Reference	Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie **83**, 75-88 (1932)

C: Hornblende (8.5 %)

Formula sum	Al5 Ca4 Fe4 H4 Mg4.37 Na1.33 O48 Si13 Ti0.14
Entry number	96-900-1227
Figure-of-Merit (FoM)	0.273509
Total number of peaks	596
Peaks in range	391
Peaks matched	107
Intensity scale factor	0.02
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 9.8030 Å b= 18.0460 Å c= 5.3130 Å β= 105.050 °
I/Ic	1.04
Calc. density	3.225 g/cm³
Reference	Phillips M. W., Draheim J. E., Popp R. K., Clowe C. A., Pinkerton A. A., "Effects of oxidation-dehydrogenation in tschermakitic hornblendesample H-11, after annealing at 650 C, 1 kbar", American Mineralogist **74**, 764-773 (1989)

D: Illite (8.5 %)

Formula sum	Al2 H2 K O12 Si4
Entry number	96-901-3719
Figure-of-Merit (FoM)	0.473215
Total number of peaks	522
Peaks in range	214
Peaks matched	98
Intensity scale factor	0.02
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.2021 Å b= 8.9797 Å c= 10.2260 Å β= 101.570 °

I/Ic	0.92
Calc. density	2.834 g/cm³
Reference	Drits V. A., Zviagina B. B., McCarty D. K., Salyn A. L., "Factors responsible for crystal-chemical variations in the solid solutionsfrom illite to aluminoceladonite and from glauconite to celadoniteLocality: Silver caldera, San Juan Mountains, ColoradoSample Name: RM30", American Mineralogist **95**, 348-361 (2010)

E: Pyrite (3.3 %)

Formula sum	Fe S2
Entry number	96-900-0596
Figure-of-Merit (FoM)	0.247681
Total number of peaks	48
Peaks in range	26
Peaks matched	5
Intensity scale factor	0.02
Space group	P 1
Crystal system	triclinic (anorthic)
Unit cell	a= 5.4166 Å b= 5.4166 Å c= 5.4166 Å α= 90.000° β= 90.000 ° γ= 90.000 °
I/Ic	3.03
Calc. density	5.014 g/cm³
Reference	Bayliss P., "Crystal structure refinement of a weakly anisotropic pyrite", American Mineralogist **62**, 1168-1172 (1977)

F: Biotite (3.1 %)

Formula sum	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13
Entry number	96-900-1583
Figure-of-Merit (FoM)	0.505691
Total number of peaks	548
Peaks in range	220
Peaks matched	55
Intensity scale factor	0.03
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 5.3350 Å b= 9.2440 Å c= 10.2060 Å β= 100.080 °
I/Ic	4.72
Calc. density	2.794 g/cm³
Reference	Bigi S., Brigatti M. F., "Crystal chemistry and microstructures of plutonic biotiteSample 1M from Valle del Cervo syenitic complex", American Mineralogist **79**, 63-72 (1994)

Candidates

Name	*Formula*	*Entry No.*	*FoM*
Selenium	Se	96-901-3138	0.6582
Periclase	Mg O	96-900-6794	0.6346
Periclase	Mg O	96-900-6751	0.6328
	Mg O	96-411-1969	0.6318
Ag Cd	Ag Cd	96-150-9174	0.6242
Rh Zr	Rh Zr	96-152-3580	0.6239
Nb Ta	Nb Ta	96-153-7943	0.6201
Periclase	Mg O	96-900-6459	0.6176
Periclase	Mg O	96-900-6752	0.6168
Periclase	Mg O	96-900-6795	0.6163
	B17 Be N2	96-210-1329	0.6155
Periclase	Mg O	96-900-0496	0.6136
Periclase	Mg O	96-900-0495	0.6135
	Fe0.91 Si0.09	96-900-6615	0.6126
(Ga0.15 Nb0.85)	Ga0.15 Nb0.85	96-152-3937	0.6119
Zn Zr	Zn Zr	96-152-7719	0.6104
(Cr0.15 Ta0.85)	Cr0.15 Ta0.85	96-152-7975	0.6104
Ru V	Ru V	96-152-7981	0.6092
Ga Ir	Ga Ir	96-152-3838	0.6089
Periclase	Mg O	96-900-6754	0.6078
	C144 Br42 Ce14 O36	96-433-0538	0.6027
Hornesite	As2 H16 Mg2.484 Ni0.516 O16	96-901-2068	0.5023
Magnesium Calcium Carbonate (.1/.9/1) (Calcite, magnesian)	C Ca0.9 Mg0.1 O3	96-721-4219	0.4702
Calcite	C Ca0.9 Mg0.1 O3	96-900-0575	0.4702
Calcite	C Ca0.871 Mg0.129 O3	96-900-1299	0.4412
Thornasite	H36 Na12 O94 Si32 Th3	96-900-2503	0.4325
Copper iron sulfide (Chalcopyrite)	Cu Fe S2	96-101-0941	0.3708
Sidwillite	H4 Mo O5	96-901-1123	0.3602
Biotite	Al2.41 Fe K4 Mg1.02 Mn0.01 Na0.07 O24 Si6 Ti0.13	96-900-1583	0.3314
Calcite	C Ca O3	96-901-4892	0.3225
Calcite	C Ca O3	96-901-4773	0.3224
Calcite	C Ca O3	96-901-5836	0.3224
Calcite	C Ca O3	96-901-6706	0.3224
Calcite	C Ca O3	96-901-6180	0.3221
Calcite	C Ca O3	96-901-4878	0.3220
Biotite	Al5 Fe6 K4 Mg3 Na0.08 O48 Si5.44 Ti	96-900-2308	0.3054
Aluminium silicate hydroxide * (Kaolinite 2M)	Al2 H4 O9 Si2	96-101-1046	0.3053
Kaolinite	Al2 O9 Si2	96-901-5000	0.3053
Calcite	C Ca O3	96-901-6707	0.2998
Calcite	C Ca O3	96-900-0967	0.2942
Buckhornite	Au Bi Pb2 S3 Te2	96-901-1521	0.2925
Calcite	C Ca O3	96-900-7690	0.2923
Calcite	C Ca O3	96-900-0966	0.2919
Calcite	C Ca O3	96-900-0968	0.2915
Calcite	C Ca O3	96-900-0096	0.2914
Calcite	C Ca O3	96-901-5391	0.2908
Calcite	C Ca O3	96-901-6023	0.2907
Calcite	C Ca O3	96-900-7688	0.2905
Calcite	C Ca O3	96-901-6465	0.2889
Calcite	C Ca O3	96-901-5482	0.2888
Calcite	C Ca O3	96-901-4612	0.2885

Calcite C Ca O3 96-901-6201 0.2884
and 122 others...

Search-Match

Settings

Reference database used	COD-Inorg REV184238 2016.07.05
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Criteria for entries added by user

Reference:

Entry number: 96-101-0930;96-101-0941;96-210-4742;96-210-4743;96-210-4753;96-210-4754;96-500-0116;96-900-0110;96-900-0595;96-900-0596;96-900-6171;96-900-6172;96-900-7573;96-901-0012;96-901-3070;96-901-3071;96-901-3072;96-901-3409;96-901-3698;96-901-5006;96-901-5235;96-901-5637;96-901-5843;96-901-6640;96-900-1665;96-900-4787;96-900-4919;96-900-7429;96-900-7612;96-900-9523;96-900-9666;96-901-0118;96-901-0494;96-901-0549;96-901-1123;96-901-1745;96-901-1746;96-901-2893;96-901-3719;96-901-3720;96-901-3721;96-901-3722;96-901-3723;96-901-3724;96-901-3733;96-901-3985;96-901-6664;96-101-1046;96-901-5000;96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707;96-100-0039;96-900-0026;96-900-0468;96-900-0469;96-900-0744;96-900-0843;96-900-0844;96-900-0845;96-900-1265;96-900-1266;96-900-1267;96-900-1268;96-900-1269;96-900-1347;96-900-1348;96-900-1349;96-900-1350;96-900-1351;96-900-1352;96-900-1353;96-900-1354;96-900-1583;96-900-1584;96-900-2302;96-900-2303;96-900-2304;96-900-2305;96-900-2306;96-900-2307;96-900-2308;96-900-1073;96-900-1226;96-900-1227;96-900-1228;96-900-1245;96-900-2503;96-900-4360;96-900-4374;96-900-4375;96-900-4376;96-900-4377;96-900-4378;96-900-4379;96-900-4380;96-900-4381;96-900-4384;96-900-4434;96-900-5257;96-900-9977;96-901-1521;96-901-2068

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0*	*FWHM*	*Matched*
1	6.78	13.0322	9.26	0.2000	
2	11.27	7.8485	8.49	0.2000	
3	11.53	7.6751	7.85	0.2000	
4	11.81	7.4947	12.96	0.2000	
5	12.08	7.3274	23.83	0.2000	
6	12.41	7.1343	59.25	0.2000	B
7	12.53	7.0646	24.93	0.2000	
8	13.18	6.7165	7.76	0.2000	
9	19.86	4.4711	26.90	0.2000	B,C,D
10	19.96	4.4484	15.64	0.2000	C,D
11	20.09	4.4195	17.97	0.2000	B,D,F
12	20.21	4.3940	13.76	0.2000	B
13	20.44	4.3459	25.53	0.2000	D
14	20.61	4.3096	24.80	0.2000	
15	20.96	4.2377	193.84	0.2000	A,B
16	21.26	4.1800	15.57	0.2000	C,F
17	21.47	4.1397	18.93	0.2000	
18	21.59	4.1162	11.43	0.2000	D
19	22.13	4.0178	9.32	0.2000	B,C
20	23.05	3.8593	9.30	0.2000	C,D
21	23.73	3.7496	8.09	0.2000	B
22	24.58	3.6219	11.52	0.2000	D,F
23	24.95	3.5687	65.93	0.2000	B
24	25.07	3.5521	24.51	0.2000	
25	25.23	3.5300	10.45	0.2000	B
26	25.39	3.5081	11.88	0.2000	B
27	26.25	3.3951	14.03	0.2000	C,F
28	26.72	3.3359	1000.00	0.2000	A,D,F
29	27.41	3.2545	8.12	0.2000	B,C
30	27.62	3.2293	10.43	0.2000	
31	29.93	2.9855	10.22	0.2000	B,C
32	30.80	2.9027	7.82	0.2000	C,D,F
33	35.02	2.5625	22.55	0.2000	B,C,D
34	35.23	2.5475	13.04	0.2000	C,D
35	35.48	2.5302	10.22	0.2000	B,F
36	35.77	2.5102	8.59	0.2000	D,F
37	36.04	2.4918	14.23	0.2000	B,D
38	36.62	2.4538	82.80	0.2000	A,C,D,F
39	37.69	2.3867	8.92	0.2000	B,C,D
40	37.99	2.3684	8.00	0.2000	C,D
41	38.50	2.3384	24.46	0.2000	B,C
42	38.67	2.3285	9.48	0.2000	C,F
43	39.53	2.2796	62.62	0.2000	A,B,C,F
44	40.38	2.2338	38.49	0.2000	A,B,C,D,F
45	42.53	2.1256	68.33	0.2000	A,B,C
46	42.69	2.1181	8.26	0.2000	B,C,D
47	45.86	1.9789	39.30	0.2000	A
48	46.03	1.9718	8.84	0.2000	B,C,D,F
49	50.21	1.8171	124.02	0.2000	A,B,D
50	50.33	1.8130	29.24	0.2000	A,C,E
51	54.76	1.6764	10.58	0.2000	B,C,D,F

52	54.93	1.6714	51.11	0.2000	A,B,C,D,F
53	55.05	1.6682	18.76	0.2000	A,D
54	55.23	1.6632	10.65	0.2000	B,D
55	55.38	1.6590	18.08	0.2000	A,B,D
56	55.48	1.6562	9.15	0.2000	A,B,D,F
57	60.01	1.5415	100.83	0.2000	A,C,D,F
58	60.17	1.5380	32.10	0.2000	A,B,C,D,F
59	61.72	1.5029	11.34	0.2000	B,C,D,E
60	61.99	1.4971	12.39	0.2000	B,C,D,E
61	62.18	1.4930	12.02	0.2000	B,C,D
62	62.35	1.4893	15.97	0.2000	B,D
63	62.47	1.4867	11.69	0.2000	B,C,D
64	62.67	1.4825	8.65	0.2000	B,C,D,F
65	63.44	1.4663	9.54	0.2000	B,C,D,F
66	64.08	1.4533	21.82	0.2000	A,B,C
67	64.24	1.4500	12.69	0.2000	A,B,C,D,E
68	67.79	1.3825	54.99	0.2000	A,C,D
69	67.98	1.3790	29.65	0.2000	A,B,C,D
70	68.18	1.3755	66.46	0.2000	A,B
71	68.36	1.3723	68.95	0.2000	A,D
72	68.55	1.3689	15.51	0.2000	A,B,C,D,F

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

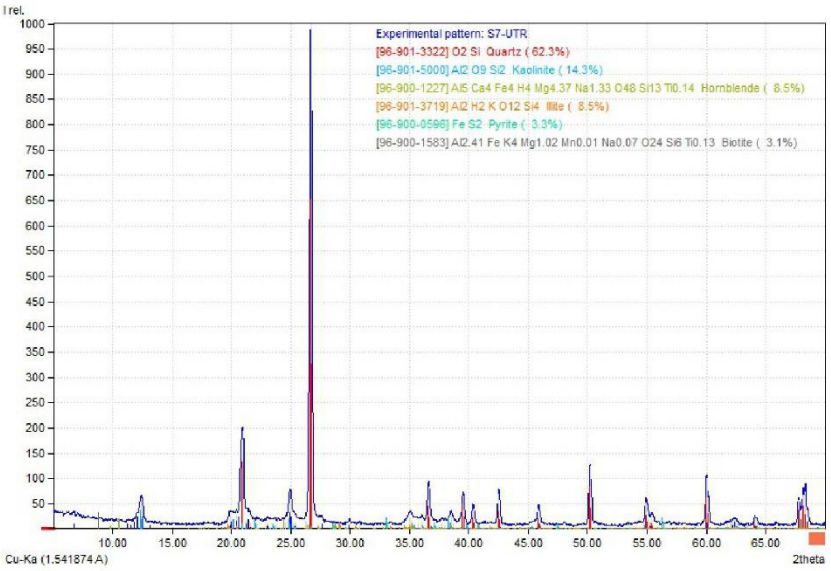
Based on calculated profile

Profile area	*Counts*	*Amount*
Overall diffraction profile	156811	100.00%
Background radiation	76350	48.69%
Diffraction peaks	80461	51.31%
Peak area belonging to selected phases	124894	79.65%
Peak area of phase A (Quartz)	*67351*	*42.95%*
Peak area of phase B (Kaolinite)	*22033*	*14.05%*
Peak area of phase C (Hornblende)	*13436*	*8.57%*
Peak area of phase D (Illite)	*11859*	*7.56%*
Peak area of phase E (Pyrite)	*4358*	*2.78%*
Peak area of phase F (Biotite)	*5857*	*3.74%*
Unidentified peak area	1883	1.20%

Peak Residuals

Peak data	*Counts*	*Amount*
Overall peak intensity	1513	100.00%
Peak intensity belonging to selected phases	454	29.98%
Unidentified peak intensity	1060	70.02%

Diffraction Pattern Graphics



C. HASIL PENGUJIAN LABORATORIUM
TOTAL SULFUR

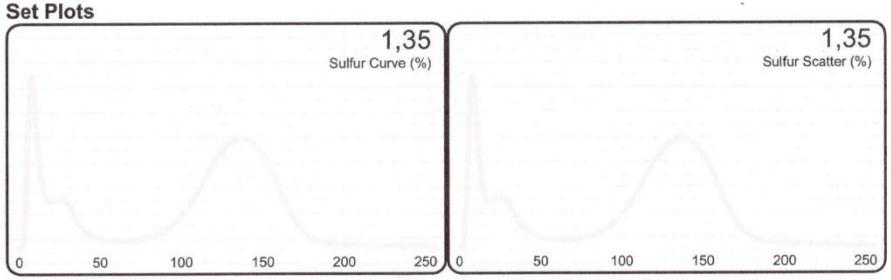
Overview

- Name: S1
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 1,35 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		1,35 %	25/04/2022 10:06:46

Set Plots



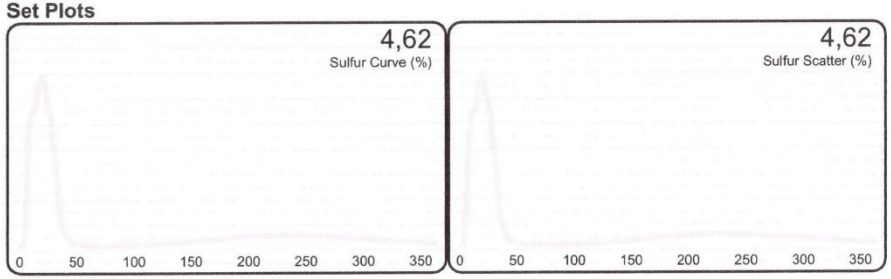
Overview

- Name: S2
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 4,62 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		4,62 %	25/04/2022 10:12:41

Set Plots



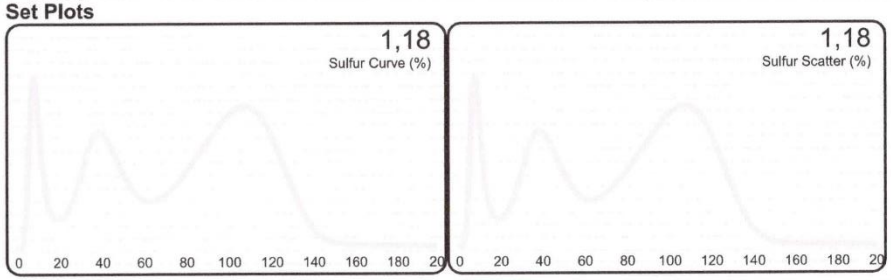
Overview

- Name: S3
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 1,18 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		1,18 %	25/04/2022 10:19:37

Set Plots



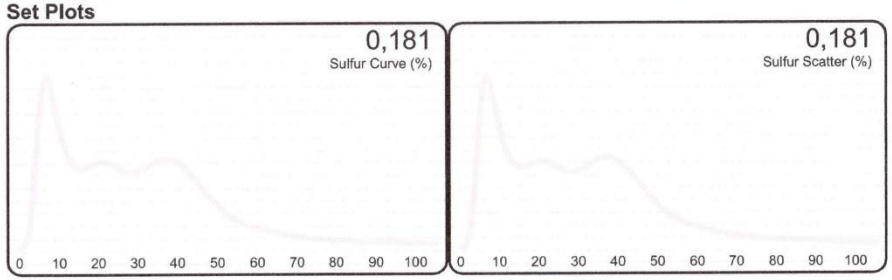
Overview

- Name: S4
- Method: BB_ADB
- Sulfur Average: 0,181 %
- Number of Included Replicates: 1
- Description:
- Sulfur Std. Dev.: 0 %
- Sulfur %RSD: 0

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		0,181 %	25/04/2022 10:24:34

Set Plots



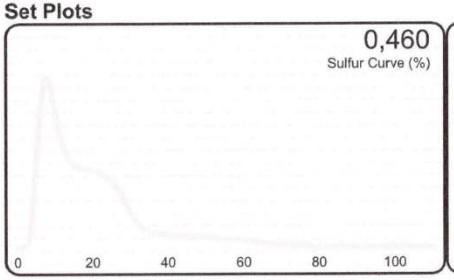
Overview

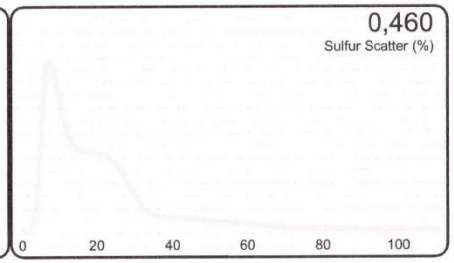
- Name: S5
- Method: BB_ADB
- Sulfur Average: 0,460 %
- Number of Included Replicates: 1
- Description:
- Sulfur Std. Dev.: 0 %
- Sulfur %RSD: 0

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		0,460 %	25/04/2022 10:27:56

Set Plots





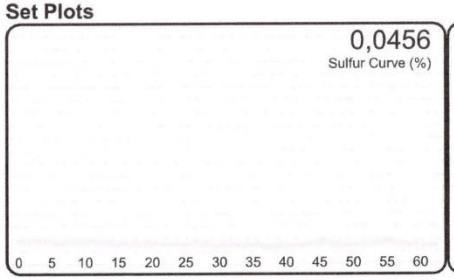
Overview

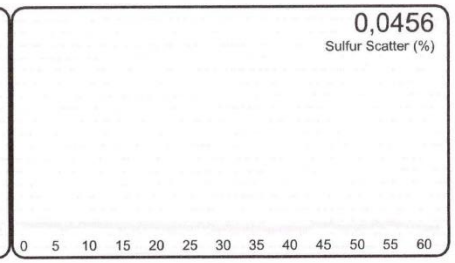
- Name: S6
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 0,0456 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		0,0456 %	25/04/2022 10:30:51

Set Plots





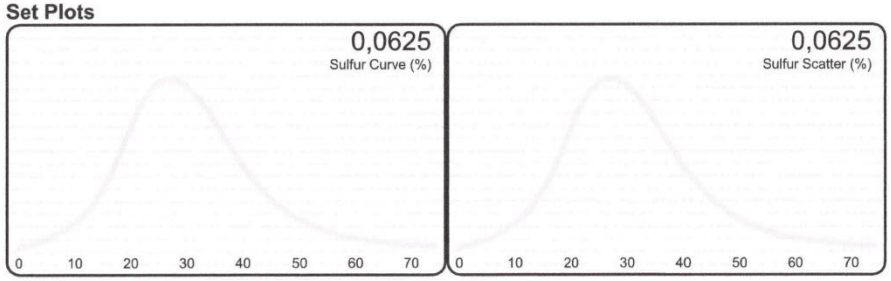
Overview

- Name: S7
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 0,0625 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		0,0625 %	25/04/2022 10:37:28

Set Plots



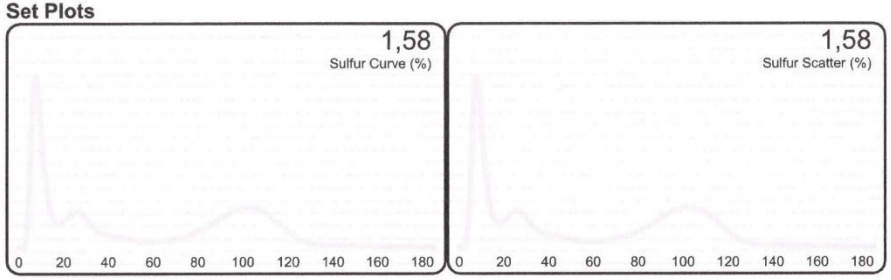
Overview

- Name: SS1
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 1,58 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		1,58 %	25/04/2022 10:40:16

Set Plots



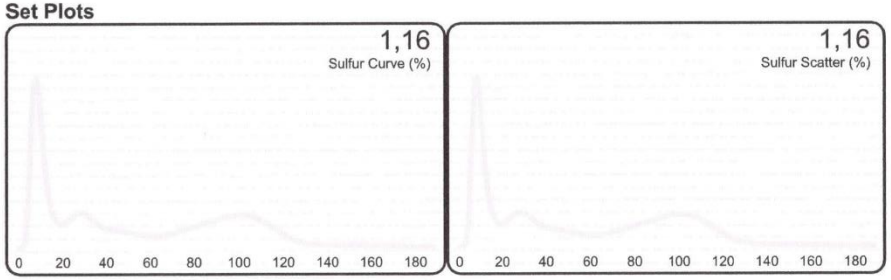
Overview

- Name: SS2
- Sulfur Std. Dev.: 0 %
- Method: BB_ADB
- Sulfur %RSD: 0
- Sulfur Average: 1,16 %
- Number of Included Replicates: 1
- Description:

Replicates

Sample Mass	Comments	Sulfur	Analysis Date
0,1000 g		1,16 %	25/04/2022 10:44:24

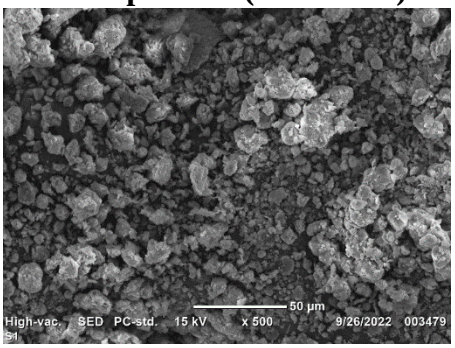
Set Plots


1,16
Sulfur Curve (%)
0 20 40 60 80 100 120 140 160 180
1,16
Sulfur Scatter (%)
0 20 40 60 80 100 120 140 160 180

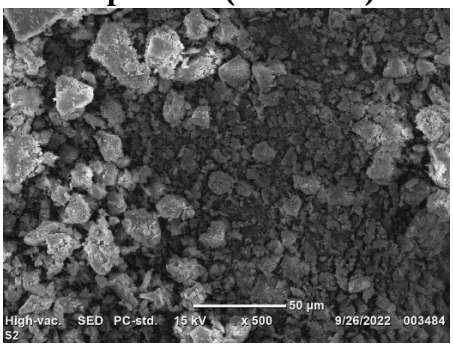
D.HASIL PENGUJIAN LABORATORIUM SEM

HASIL SCANNING ELECTRON MICROSCOPE (SEM)
PEMBESARAN 500

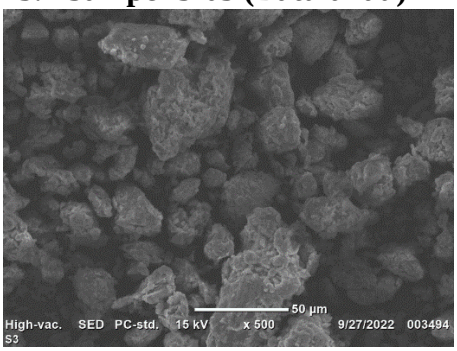
1. Sampel S-01 (Batulanau)



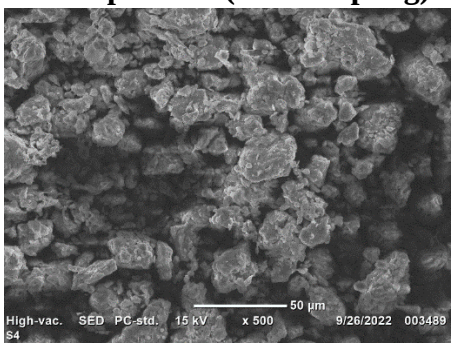
2. Sampel S-02 (Batubara)



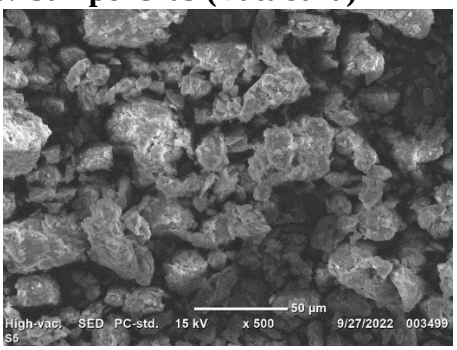
3. Sampel S-03 (Batulanau)



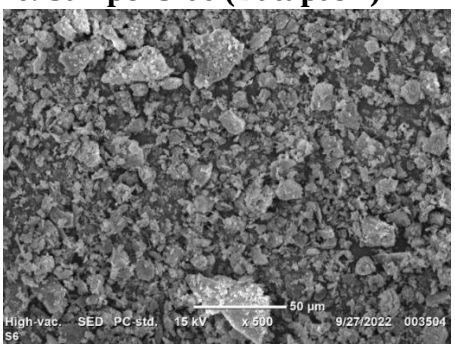
5. Sampel S-04 (Batulempung)



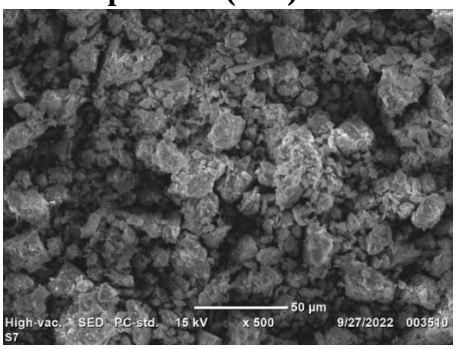
5. Sampel S-05 (Batubara)



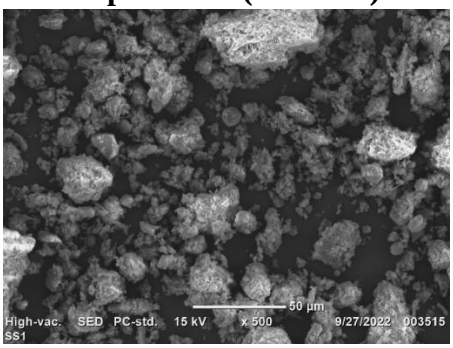
6. Sampel S-06 (Batupasir)



7. Sampel S-07 (Soil)

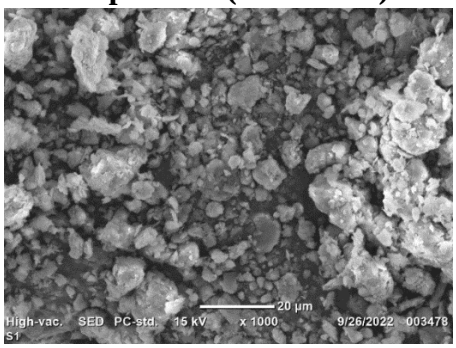


8. Sampel SS-01 (Sedimen)

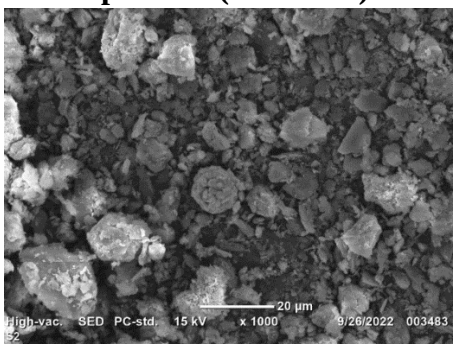


HASIL SCANNING ELECTRON MICROSCOPE (SEM)
PEMBESARAN 1000

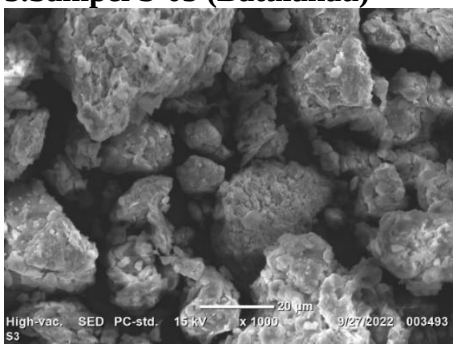
1. Sampel S-01 (Batulanau)



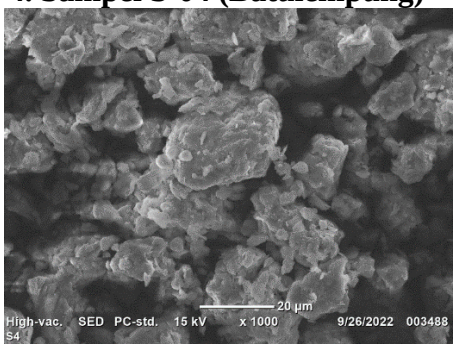
2. Sampel S-02 (Batubara)



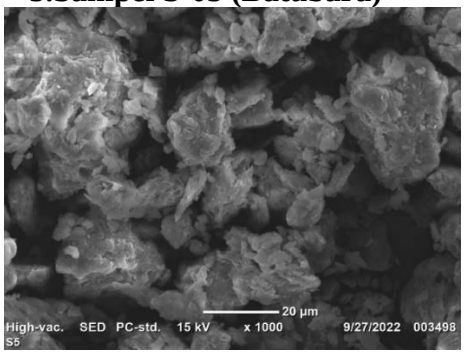
3.Sampel S-03 (Batulanau)



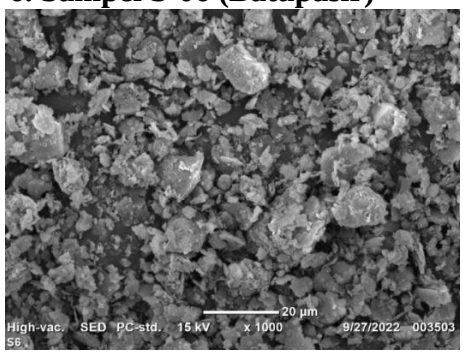
4. Sampel S-04 (Batulempung)



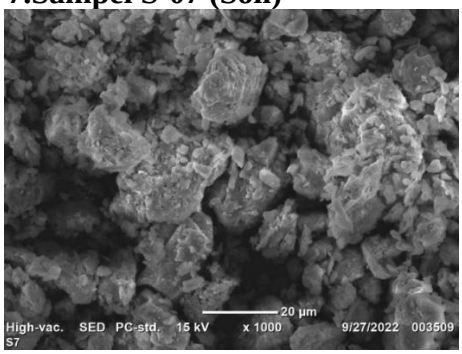
5.Sampel S-05 (Batubara)



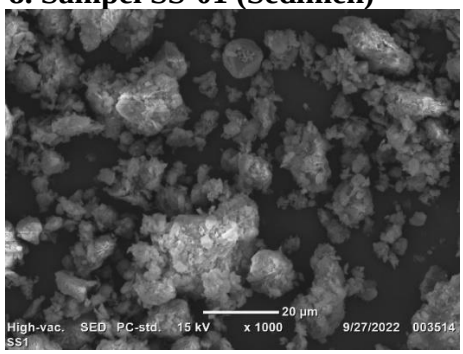
6. Sampel S-06 (Batupasir)



7.Sampel S-07 (Soil)

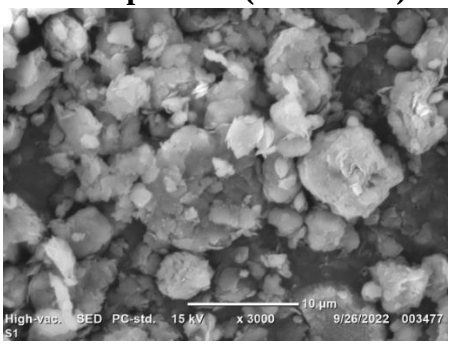


8. Sampel SS-01 (Sedimen)

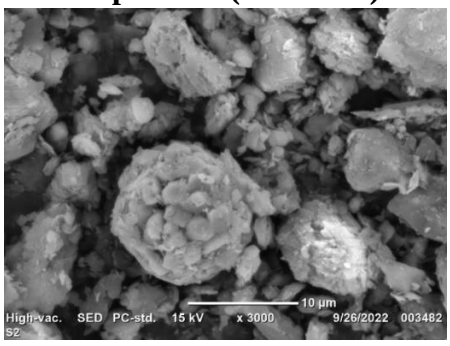


HASIL SCANNING ELECTRON MICROSCOPE (SEM) PEMBESARAN 3000

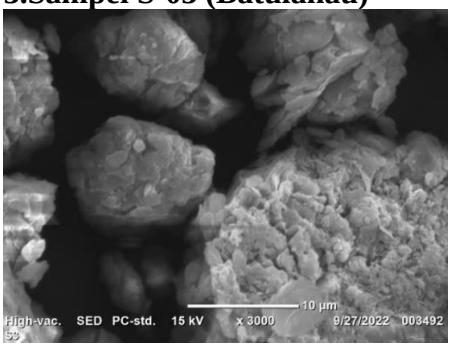
1. Sampel S-01 (Batulanau)



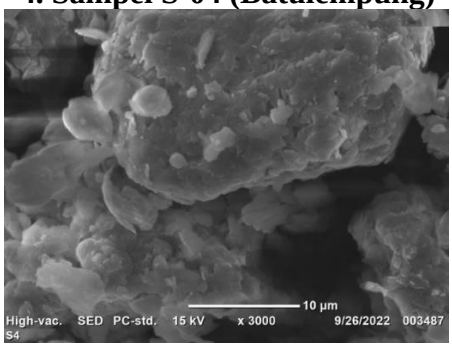
2. Sampel S-02 (Batubara)



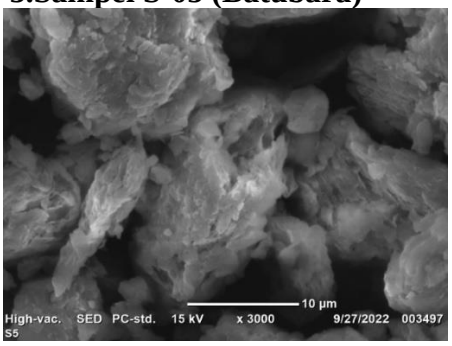
3.Sampel S-03 (Batulanau)



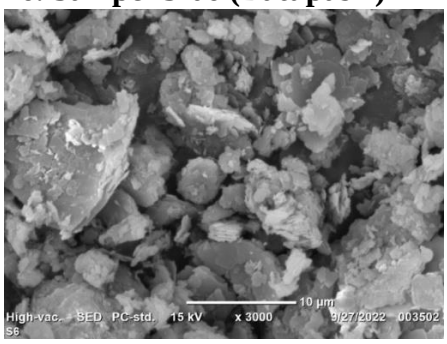
4. Sampel S-04 (Batulempung)



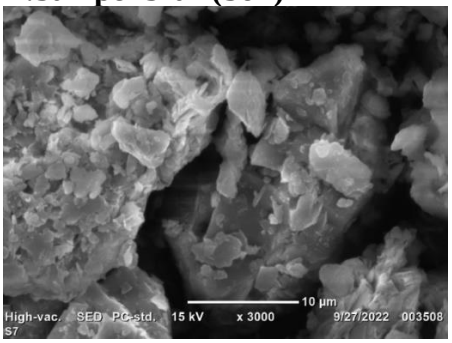
5.Sampel S-05 (Batubara)



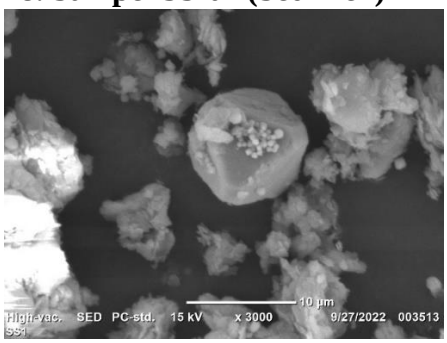
6. Sampel S-06 (Batupasir)



7.Sampel S-07 (Soil)

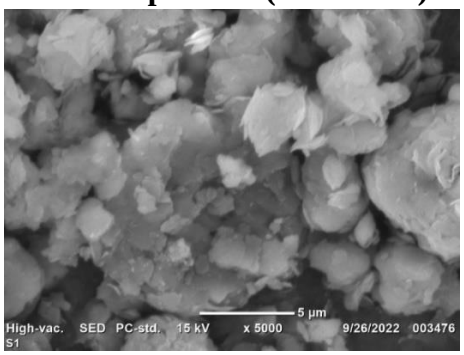


8. Sampel SS-01 (Sedimen)

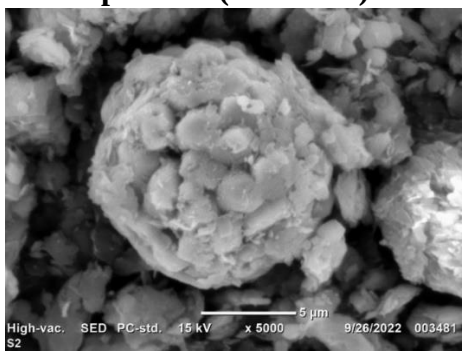


HASIL SCANNING ELECTRON MICROSCOPE (SEM) PEMBESARAN 5000

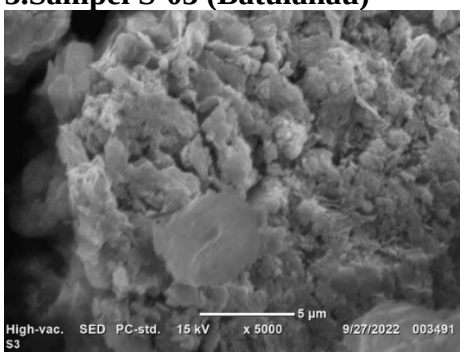
1. Sampel S-01 (Batulanau)



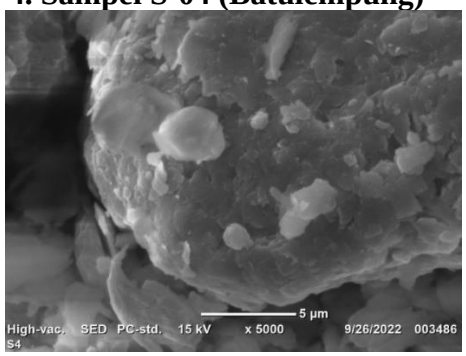
2. Sampel S-02 (Batubara)



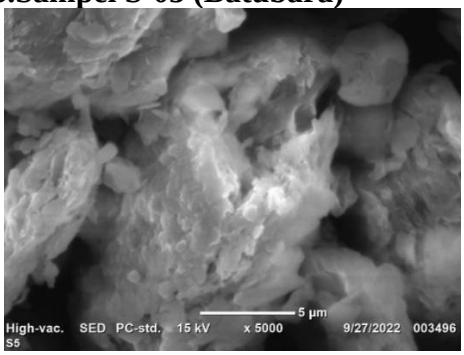
3.Sampel S-03 (Batulanau)



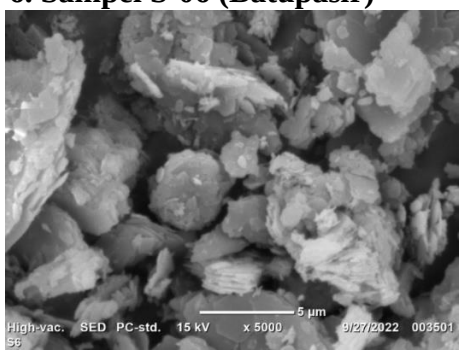
4. Sampel S-04 (Batulempung)



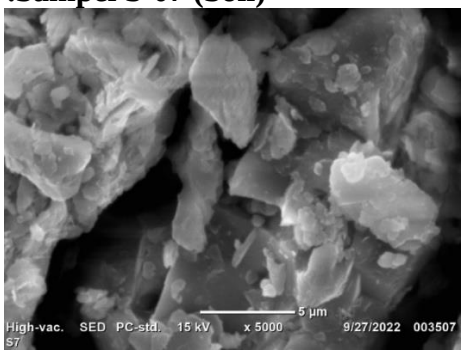
5.Sampel S-05 (Batubara)



6. Sampel S-06 (Batupasir)



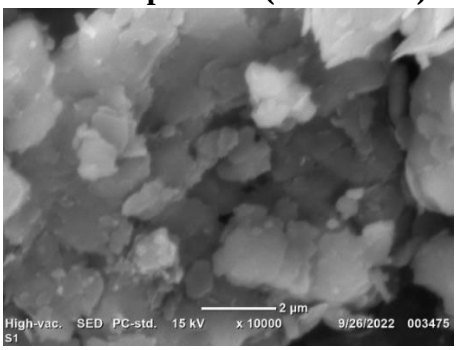
7.Sampel S-07 (Soil)



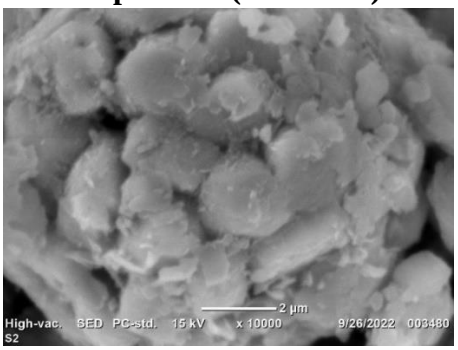
8. Sampel SS-01 (Sedimen)

HASIL SCANNING ELECTRON MICROSCOPE (SEM) PEMBESARAN 10000

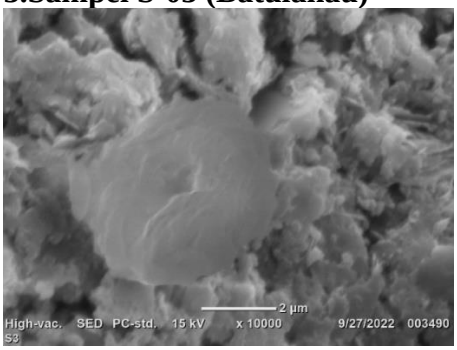
1. Sampel S-01 (Batulanau)



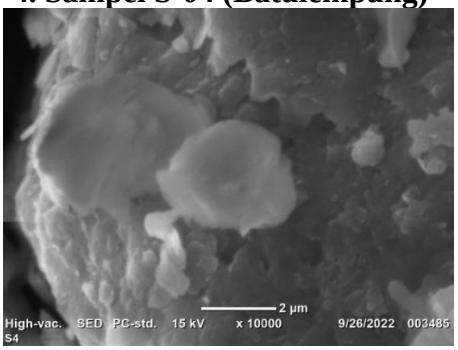
2. Sampel S-02 (Batubara)



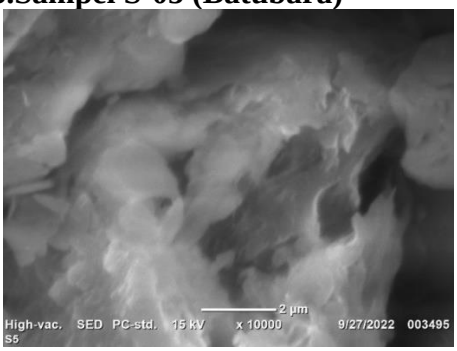
3.Sampel S-03 (Batulanau)



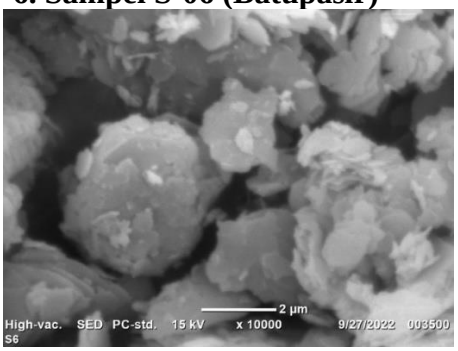
4. Sampel S-04 (Batulempung)



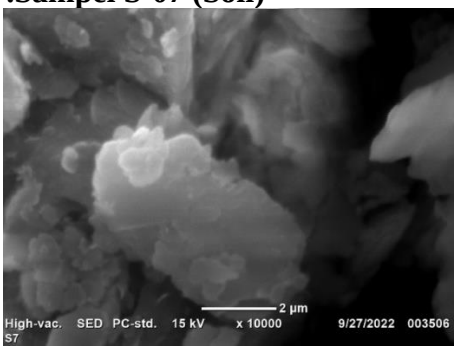
5.Sampel S-05 (Batubara)



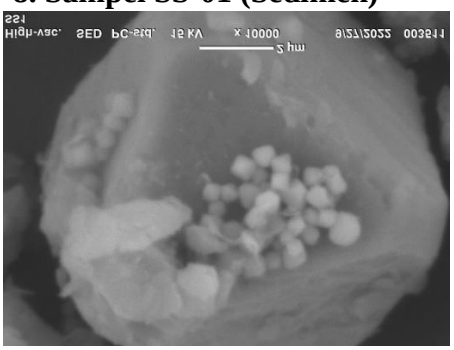
6. Sampel S-06 (Batupasir)



7.Sampel S-07 (Soil)

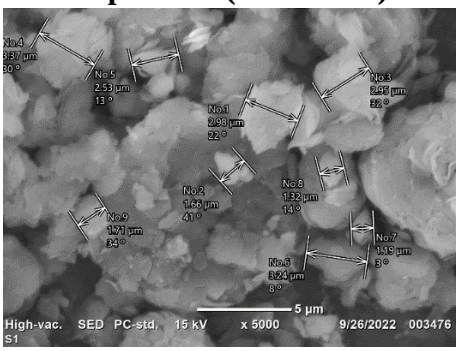


8. Sampel SS-01 (Sedimen)

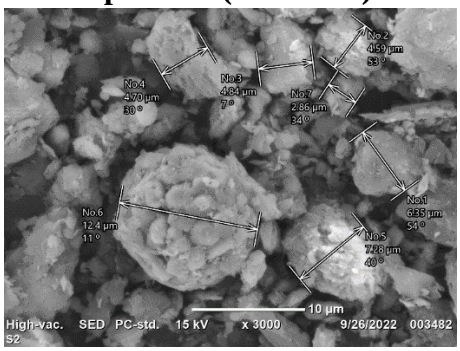


HASIL SCANNING ELECTRON MICROSCOPE (SEM) UKURAN PARTIKEL

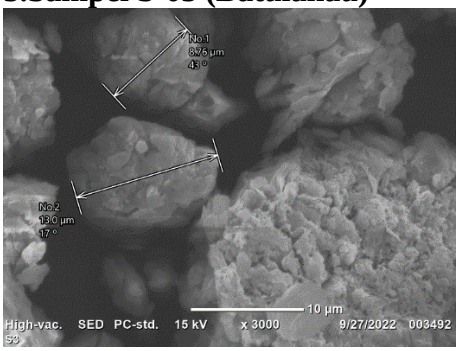
1. Sampel S-01 (Batulanau)



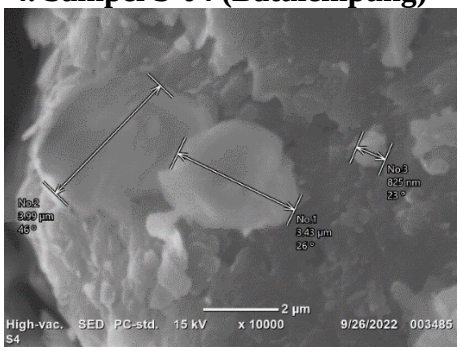
2. Sampel S-02 (Batubara)



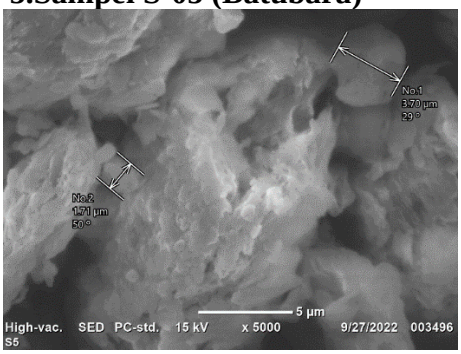
3.Sampel S-03 (Batulanau)



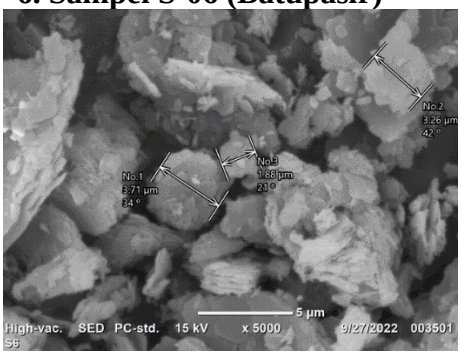
4. Sampel S-04 (Batulempung)



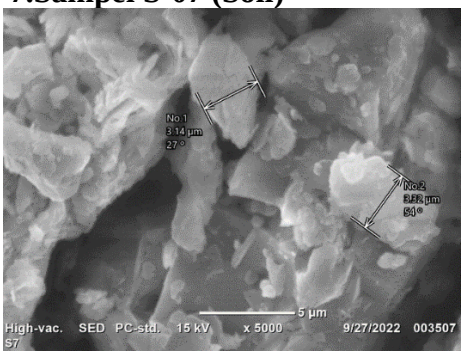
5.Sampel S-05 (Batubara)



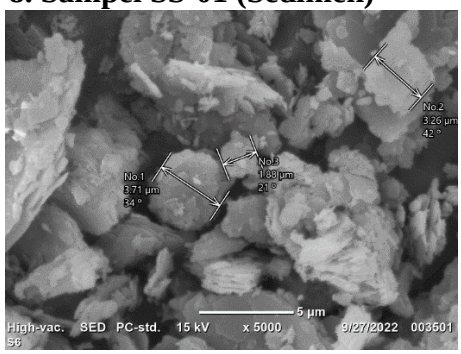
6. Sampel S-06 (Batupasir)



7.Sampel S-07 (Soil)



8. Sampel SS-01 (Sedimen)



E. HASIL PENGUJIAN LABORATORIUM ANALISIS KINETIK METODE FDCLT

TABEL UJI KINETIK (FDCL) PRIODE PERHARI							
NO	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	06/09/2022	S-01 (Batulanau)	300	200	73	6,7	26
2		S-02 (Batubara)	300	200	98	5,2	26
3		S-03 (Batulanau)	300	200	90	1,9	26
4		S-04 (Batulempung)	300	200	45	4,1	26
5		S-05 (Batubara)	300	200	120	6,3	26
6	07/09/2022	S-01 (Batulanau)	300	200	125	7,3	25
7		S-02 (Batubara)	300	200	140	6,8	25
8		S-03 (Batulanau)	300	200	175	2,4	25
9		S-04 (Batulempung)	300	200	75	5,1	25
10		S-05 (Batubara)	300	200	150	5,2	25
11	08/09/2022	S-01 (Batulanau)	300	200	165	7,2	26
12		S-02 (Batubara)	300	200	190	5,3	24
13		S-03 (Batulanau)	300	200	175	2,3	24
14		S-04 (Batulempung)	300	200	130	4,1	24
15		S-05 (Batubara)	300	200	125	5,4	24
16	09/09/2022	S-01 (Batulanau)	300	200	130	7,4	25
17		S-02 (Batubara)	300	200	125	7,7	25
18		S-03 (Batulanau)	300	200	155	2,6	25
19		S-04 (Batulempung)	300	200	110	4,3	25
20		S-05 (Batubara)	300	200	150	5,3	25
21	10/09/2022	S-01 (Batulanau)	300	200	140	8,7	25
22		S-02 (Batubara)	300	200	125	7,7	25
23		S-03 (Batulanau)	300	200	150	2,4	25
24		S-04 (Batulempung)	300	200	155	3,6	25
25		S-05 (Batubara)	300	200	170	5,3	25
26	11/09/2022	S-01 (Batulanau)	300	200	135	8,5	25
27		S-02 (Batubara)	300	200	175	6,4	25
28		S-03 (Batulanau)	300	200	160	2,4	25
29		S-04 (Batulempung)	300	200	170	3,7	26
30		S-05 (Batubara)	300	200	160	4,6	25
31	12/09/2022	S-01 (Batulanau)	300	200	110	7,7	25
32		S-02 (Batubara)	300	200	160	7,1	25
33		S-03 (Batulanau)	300	200	165	2,3	25
34		S-04 (Batulempung)	300	200	140	3,8	25
35		S-05 (Batubara)	300	200	100	5,9	24
36	13/09/2022	S-01 (Batulanau)	300	200	125	7,5	25
37		S-02 (Batubara)	300	200	160	6,4	25
38		S-03 (Batulanau)	300	200	190	2,3	25
39		S-04 (Batulempung)	300	200	175	3,9	24
40		S-05 (Batubara)	300	200	190	5,6	24
41	14/09/2022	S-01 (Batulanau)	300	200	125	7,1	25
42		S-02 (Batubara)	300	200	170	6,8	25

NO	Sampel	Sampel	Berat (gr)	Air (ml)	Air Lindi (ml)	pH	Suhu (C)
43		S-03 (Batulanau)	300	200	145	2,3	25
44		S-04 (Batulempung)	300	200	145	4,1	25
45		S-05 (Batubara)	300	200	155	5,0	24
46	15/09/2022	S-01 (Batulanau)	300	200	120	7,2	25
47		S-02 (Batubara)	300	200	130	7,0	25
48		S-03 (Batulanau)	300	200	150	2,4	25
49		S-04 (Batulempung)	300	200	150	3,6	24
50		S-05 (Batubara)	300	200	120	4,7	24
51	16/09/2022	S-01 (Batulanau)	300	200	150	7,0	25
52		S-02 (Batubara)	300	200	175	7,2	26
53		S-03 (Batulanau)	300	200	130	2,4	25
54		S-04 (Batulempung)	300	200	175	3,7	25
55		S-05 (Batubara)	300	200	150	4,8	25
56	17/09/2022	S-01 (Batulanau)	300	200	150	7,0	25
57		S-02 (Batubara)	300	200	175	7,1	26
58		S-03 (Batulanau)	300	200	180	2,4	25
59		S-04 (Batulempung)	300	200	140	3,8	25
60		S-05 (Batubara)	300	200	150	4,9	25
61	18/09/2022	S-01 (Batulanau)	300	200	150	7,3	25
62		S-02 (Batubara)	300	200	125	7,4	25
63		S-03 (Batulanau)	300	200	150	2,6	25
64		S-04 (Batulempung)	300	200	175	3,9	25
65		S-05 (Batubara)	300	200	150	5,3	25
66	19/09/2022	S-01 (Batulanau)	300	200	150	7,4	23
67		S-02 (Batubara)	300	200	140	7,3	23
68		S-03 (Batulanau)	300	200	125	2,7	23
69		S-04 (Batulempung)	300	200	150	3,7	23
70		S-05 (Batubara)	300	200	140	5,1	23

TABEL UJI KINETIK (FDCL) PRIODE PERPEKAN							
No	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	27/09/2022	S-01 (Batulanau)	300	200	73	6,7	26
2		S-02 (Batubara)	300	200	98	5,9	26
3		S-03 (Batulanau)	300	200	90	1,9	26
4		S-04 (Batulempung)	300	200	45	4,1	26
5		S-05 (Batubara)	300	200	120	6,3	26
6	04/10/2022	S-01 (Batulanau)	300	200	125	7,3	25
7		S-02 (Batubara)	300	200	140	5,8	25
8		S-03 (Batulanau)	300	200	175	2,4	25
9		S-04 (Batulempung)	300	200	75	5,1	25
10		S-05 (Batubara)	300	200	150	5,2	25

TABEL UJI KINETIK (FDCL) PRIODE PERBULAN							
No	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	04/11/2022	S-01 (Batulanau)	300	200	73	6,7	26.1
2		S-02 (Batubara)	300	200	98	5,8	26.1
3		S-03 (Batulanau)	300	200	90	1,9	26.1
4		S-04 (Batulempung)	300	200	45	4,1	26.1
5		S-05 (Batubara)	300	200	120	6,3	26.1
6	06/12/2022	S-01 (Batulanau)	300	200	125	7,3	25
7		S-02 (Batubara)	300	200	140	5,7	25
8		S-03 (Batulanau)	300	200	175	2,4	25
9		S-04 (Batulempung)	300	200	75	5,1	25
10		S-05 (Batubara)	300	200	150	5,2	25

TABEL UJI KINETIK (FDCL) PRIODE PERHARI							
NO	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	**08/12/2022**	SS-1 (Sedimen)	300	200	175	7,5	26
2		S-06 (Batupasir)	300	200	175	6,5	26
3		S-07 (Top Soil)	300	200	175	6,3	26
4	**09/12/2022**	SS-1 (Sedimen)	300	200	170	7,7	25
5		S-06 (Batupasir)	300	200	160	6,4	25
6		S-07 (Top Soil)	300	200	170	6,4	25
7	**10/12/2022**	SS-1 (Sedimen)	300	200	170	7,0	26
8		S-06 (Batupasir)	300	200	170	6,9	24
9		S-07 (Top Soil)	300	200	160	6,5	24
10	**11/12/2022**	SS-1 (Sedimen)	300	200	170	7,2	25
11		S-06 (Batupasir)	300	200	170	6,7	25
12		S-07 (Top Soil)	300	200	160	6,4	25
13	**12/12/2022**	SS-1 (Sedimen)	300	200	160	7,3	25
14		S-06 (Batupasir)	300	200	170	6,3	25
15		S-07 (Top Soil)	300	200	170	6,8	25
16	**13/12/2022**	SS-1 (Sedimen)	300	200	160	7,5	25
17		S-06 (Batupasir)	300	200	180	6,5	25
18		S-07 (Top Soil)	300	200	180	6,9	26
19	**14/12/2022**	SS-1 (Sedimen)	300	200	170	7,6	25
20		S-06 (Batupasir)	300	200	180	6,7	25
21		S-07 (Top Soil)	300	200	180	7,1	25
22	**15/12/2022**	SS-1 (Sedimen)	300	200	170	7,7	25
23		S-06 (Batupasir)	300	200	180	6,9	25
24		S-07 (Top Soil)	300	200	180	6,9	24
25	**16/12/2022**	SS-1 (Sedimen)	300	200	170	7,1	25
26		S-06 (Batupasir)	300	200	180	6,8	25
27		S-07 (Top Soil)	300	200	175	7,2	25
28	**17/12/2022**	SS-1 (Sedimen)	300	200	165	7,3	25
29		S-06 (Batupasir)	300	200	175	6,9	25
30		S-07 (Top Soil)	300	200	180	7,2	24
31	**18/12/2022**	SS-1 (Sedimen)	300	200	160	7,0	25
32		S-06 (Batupasir)	300	200	180	6,8	25
33		S-07 (Top Soil)	300	200	175	7,0	25
34	**19/12/2022**	SS-1 (Sedimen)	300	200	160	7,1	25
35		S-06 (Batupasir)	300	200	175	7,0	25
36		S-07 (Top Soil)	300	200	175	7,2	25
37	**20/12/2022**	SS-1 (Sedimen)	300	200	160	7,3	25
38		S-06 (Batupasir)	300	200	175	7,0	25
39		S-07 (Top Soil)	300	200	175	7,1	25
40	**21/12/2022**	SS-1 (Sedimen)	300	200	160	7,1	23
41		S-06 (Batupasir)	300	200	180	7,0	23
42		S-07 (Top Soil)	300	200	185	6,8	23

TABEL UJI KINETIK (FDCL) PRIODE PERPEKAN							
NO	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	**28/12/2022**	SS-1 (Sedimen)	300	200	160	7,1	26
2		S-06 (Batupasir)	300	200	190	7,0	26
3		S-07 (Top Soil)	300	200	185	6,8	26
4	**04/01/2023**	SS-1 (Sedimen)	300	200	160	7,0	26
5		S-06 (Batupasir)	300	200	180	7,0	26
6		S-07 (Top Soil)	300	200	175	6,9	26

TABEL UJI KINETIK (FDCL) PRIODE PERBULAN							
NO	**Sampel**	**Sampel**	**Berat (gr)**	**Air (ml)**	**Air Lindi (ml)**	**pH**	**Suhu (C)**
1	**02/02/2023**	SS-1 (Sedimen)	300	200	180	7,0	26
2		S-06 (Batupasir)	300	200	180	6,9	26
3		S-07 (Top Soil)	300	200	175	7,1	26
4	**04/03/2023**	SS-1 (Sedimen)	300	200	180	7,0	26
5		S-06 (Batupasir)	300	200	190	7,0	26
6		S-07 (Top Soil)	300	200	185	6,8	26