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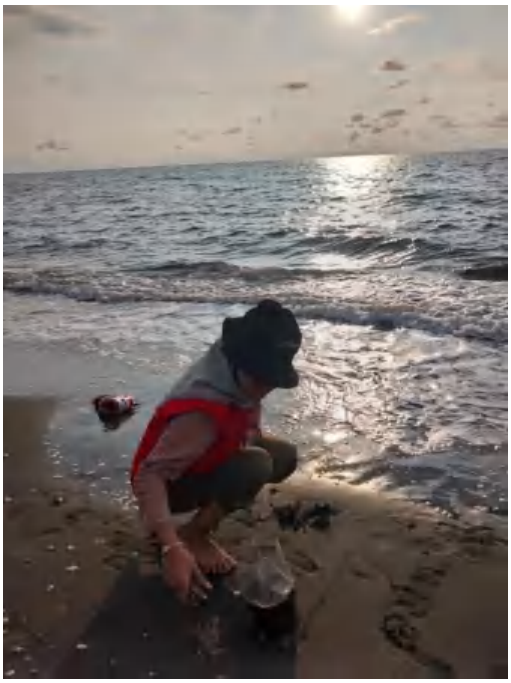
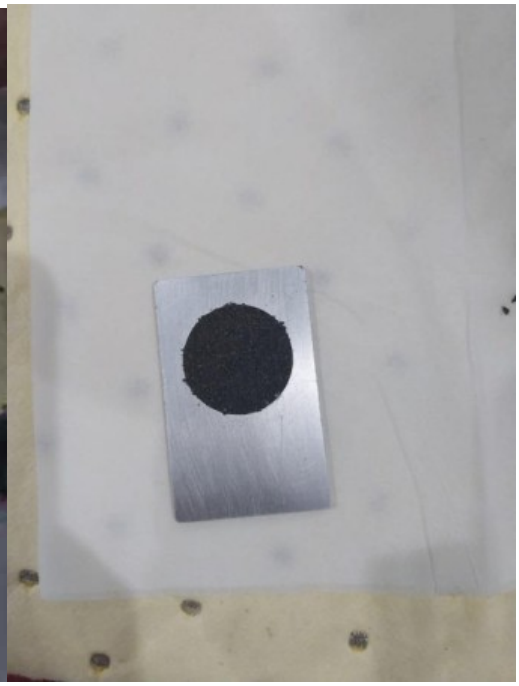
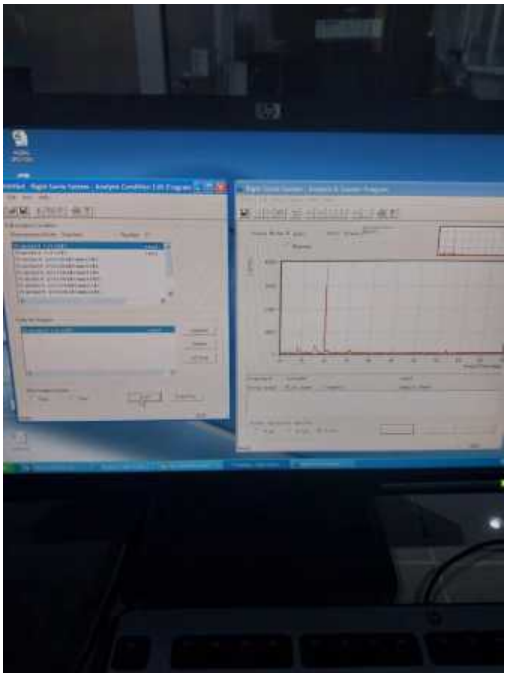
LAMPIRAN

DOKUMENTASI PENGAMBILAN SAMPEL

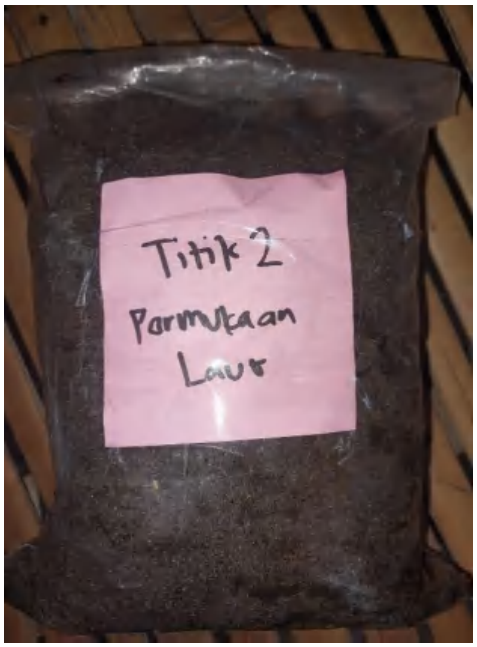


PROSES ANALISIS MENGGUNAKAN *X-RAY DIFFRACTION*





SAMPEL PENELITIAN



ALAT DAN BAHAN BAHAN






1. **Hasil metode XRD untuk sampel titik 1**

Match! Phase Analysis Report

Sample: sand ()

Sample Data

File name	titik#1.RAW
File path	C:/Program Files/Match3/geofisika/titik#1
Data collected	Jan 25, 2024 16:11:26
Data range	20.440º - 70.440º
Original data range	20.000º - 70.000º
Number of points	2501
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	No
2theta correction	0.44º
Radiation	X-rays
Wavelength	1.540600 Å

ndex	***Amount (%)***	***Name***	***Formula sum***
A	26.6	Potassium [iron(II)/magnesium] iron(III) bis(orthophosphate)	Fe1.91 K Mg0.09 O8 P2
B	73.4		Ba Fe2 H6 O17 P4
	38.5	*Unidentified peak area*	

Element	***Amount (weight %)***
O	*40.7%(*)*
Fe	21.0%
P	18.8%
Ba	15.5%
K	3.1%
H	*0.7%(*)*
Mg	0.2%
**LE (sum)*	*41.4%*

Details of identified phases

A: Potassium [iron(II)/magnesium] iron(III) bis(orthophosphate) (26.6 %)*

Formula sum	Fe1.91 K Mg0.09 O8 P2
Entry number	96-223-5287
Figure-of-Merit (FoM)	0.731264*
Total number of peaks	500
Peaks in range	282
Peaks matched	192
Intensity scale factor	0.19
2theta correction	0.063°
Space group	P 1 21/n 1
tem	Monoclinic
	a= 7.8444 Å b= 10.0033 Å c= 9.0371 Å β= 114.838 º
	2.36
ty	3.488 g/cm³
	light pink
	Yatskin Michael M., Zatovsky Igor V., Baumer Vyacheslav N., Ogorodnyk Ivan V., Slobodyanik Nikolay S.,

"KMg~0.09~Fe~1.91~(PO~4~)~2~", Acta Crystallographica Section E **68(6)**, i51 (2012)

B: Ba Fe2 H6 O17 P4 (73.4 %)*

Formula sum	Ba Fe2 H6 O17 P4
Entry number	96-156-3020
Figure-of-Merit (FoM)	0.781148*
Total number of peaks	499
Peaks in range	271
Peaks matched	181
Intensity scale factor	0.46
2theta correction	-0.002°
Space group	P 1 21/c 1
Crystal system	Monoclinic
Unit cell	a= 9.4956 Å b= 7.8990 Å c= 9.4444 Å β= 117.498 °
I/Ic	2.06
Calc. density	3.441 g/cm³
Color	Yellow
Reference	Sun Wei, Huang Ya-Xi, Pan Yuanming, Mi Jin-Xiao, "Investigation on pseudosymmetry, twinning and disorder in crystalstructure determinations: Ba(H2O)M2III[PO3(OH)]4 (M=Fe, V) as examples", Journal of Solid State Chemistry **187**, 89-96 (2012)

(*)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Search-Match

Settings

Reference database used	COD-Inorg 2023.12.05
Automatic zeropoint adaptation	Yes
Downgrade entries with low scaling factors	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	0
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Selection Criteria

Elements:

Elements that must be present: Fe

Elements that may be present: All elements not mentioned above

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0 (peak height)*	*Counts (peak area)*	*FWHM*	*Matched*
	24.62	3.6130	52.50	6.44	0.1200	A,B
	26.46	3.3658	9.43	1.16	0.1200	A
	26.70	3.3361	10.62	2.61	0.2400	A
	27.36	3.2571	6.06	0.99	0.1600	
	27.58	3.2316	5.23	0.21	0.0400	
	27.78	3.2088	7.90	0.32	0.0400	B
	28.66	3.1122	46.45	15.20	0.3200	

8	29.06	3.0703	59.52	4.87	0.0800	A,B
9	29.20	3.0559	62.76	12.83	0.2000	B
10	30.36	2.9417	7.68	0.31	0.0400	
11	30.70	2.9099	14.62	2.39	0.1600	A,B
12	31.24	2.8608	1000.00	122.71	0.1200	A,B
13	31.78	2.8135	12.91	1.06	0.0800	B
14	32.24	2.7744	3.44	0.28	0.0800	
15	32.68	2.7380	6.68	0.55	0.0800	A
16	33.24	2.6931	6.25	0.26	0.0400	A
17	34.00	2.6347	4.25	0.17	0.0400	A,B
18	35.84	2.5035	11.06	0.90	0.0800	A,B
19	36.02	2.4914	6.58	0.27	0.0400	A,B
20	36.36	2.4689	58.03	7.12	0.1200	
21	36.66	2.4494	15.55	2.54	0.1600	A,B
22	37.30	2.4088	3.71	0.15	0.0400	A,B
23	37.58	2.3915	3.49	0.29	0.0800	A
24	38.64	2.3283	4.31	0.88	0.2000	A,B
25	39.22	2.2952	3.59	0.44	0.1200	A,B
26	39.76	2.2652	3.64	0.30	0.0800	A,B
27	41.50	2.1742	3.25	0.40	0.1200	A,B
28	41.76	2.1613	36.86	4.52	0.1200	A,B
29	42.44	2.1282	4.76	0.39	0.0800	A
30	43.58	2.0751	8.19	0.67	0.0800	B
31	43.82	2.0643	3.91	0.16	0.0400	A
32	47.32	1.9195	3.70	0.15	0.0400	A,B
33	49.02	1.8568	3.61	0.15	0.0400	A,B
34	49.28	1.8476	35.30	2.89	0.0800	A,B
35	49.68	1.8337	4.11	0.50	0.1200	A,B
36	50.00	1.8227	2.99	0.37	0.1200	A,B
37	50.16	1.8172	5.62	0.23	0.0400	B
38	50.42	1.8085	8.55	0.35	0.0400	A,B
39	51.56	1.7711	7.86	0.32	0.0400	A,B
40	51.76	1.7648	14.91	1.83	0.1200	B
41	52.02	1.7566	10.64	0.44	0.0400	A,B
42	52.22	1.7503	4.77	0.20	0.0400	A,B
43	52.42	1.7441	16.44	1.34	0.0800	A
44	52.58	1.7392	13.54	0.55	0.0400	A,B
45	53.14	1.7221	3.01	0.49	0.1600	A,B
46	57.92	1.5909	5.36	1.10	0.2000	A,B
47	58.12	1.5859	4.22	0.35	0.0800	A,B
48	58.30	1.5814	4.49	0.73	0.1600	A,B
49	58.90	1.5667	53.31	6.54	0.1200	A,B
50	59.08	1.5624	22.86	0.94	0.0400	A
51	59.34	1.5561	3.75	0.15	0.0400	A,B
52	60.04	1.5397	3.66	0.15	0.0400	A,B
53	60.90	1.5200	4.65	0.19	0.0400	A,B
54	61.26	1.5119	3.95	0.16	0.0400	A,B
55	61.80	1.5000	2.98	0.49	0.1600	A,B
56	62.06	1.4943	7.77	0.64	0.0800	A,B
57	62.26	1.4900	4.12	0.34	0.0800	A,B
58	62.58	1.4831	6.40	0.52	0.0800	A,B
59	62.76	1.4793	11.00	0.90	0.0800	B
60	62.90	1.4764	11.78	1.93	0.1600	A,B
61	63.04	1.4734	9.64	1.18	0.1200	A,B
62	63.38	1.4663	9.77	1.20	0.1200	A,B
	63.94	1.4548	4.91	0.20	0.0400	A,B
	64.10	1.4516	5.52	0.23	0.0400	A
	64.26	1.4484	6.41	0.79	0.1200	A,B
	64.52	1.4432	10.57	0.86	0.0800	A
	64.66	1.4404	8.10	1.66	0.2000	A,B
	64.94	1.4348	7.74	0.32	0.0400	A,B
	65.10	1.4317	5.06	0.21	0.0400	A,B

70	65.26	1.4286	3.73	0.15	0.0400	A
71	65.44	1.4251	6.19	0.51	0.0800	A
72	65.68	1.4204	7.61	0.31	0.0400	B
73	66.00	1.4143	8.60	0.70	0.0800	A,B
74	66.26	1.4094	5.55	0.23	0.0400	A,B
75	66.42	1.4064	7.24	0.30	0.0400	A,B
76	66.56	1.4038	6.56	1.34	0.2000	A,B
77	66.84	1.3986	5.88	0.48	0.0800	A,B
78	66.98	1.3960	7.03	0.29	0.0400	B
79	67.28	1.3905	5.72	0.23	0.0400	A,B
80	67.78	1.3815	5.68	0.23	0.0400	A,B
81	68.00	1.3775	5.11	0.21	0.0400	A,B
82	68.22	1.3736	5.87	0.48	0.0800	A,B
83	68.40	1.3704	9.28	1.14	0.1200	A,B
84	68.68	1.3655	7.30	0.90	0.1200	A,B
85	68.92	1.3614	8.10	0.33	0.0400	A,B
86	69.10	1.3583	5.75	0.24	0.0400	A,B
87	69.36	1.3538	17.09	2.10	0.1200	A,B
88	69.54	1.3507	9.91	1.22	0.1200	A,B
89	69.78	1.3467	3.79	0.46	0.1200	B
90	70.00	1.3430	3.32	0.41	0.1200	A,B

Integrated Profile Areas

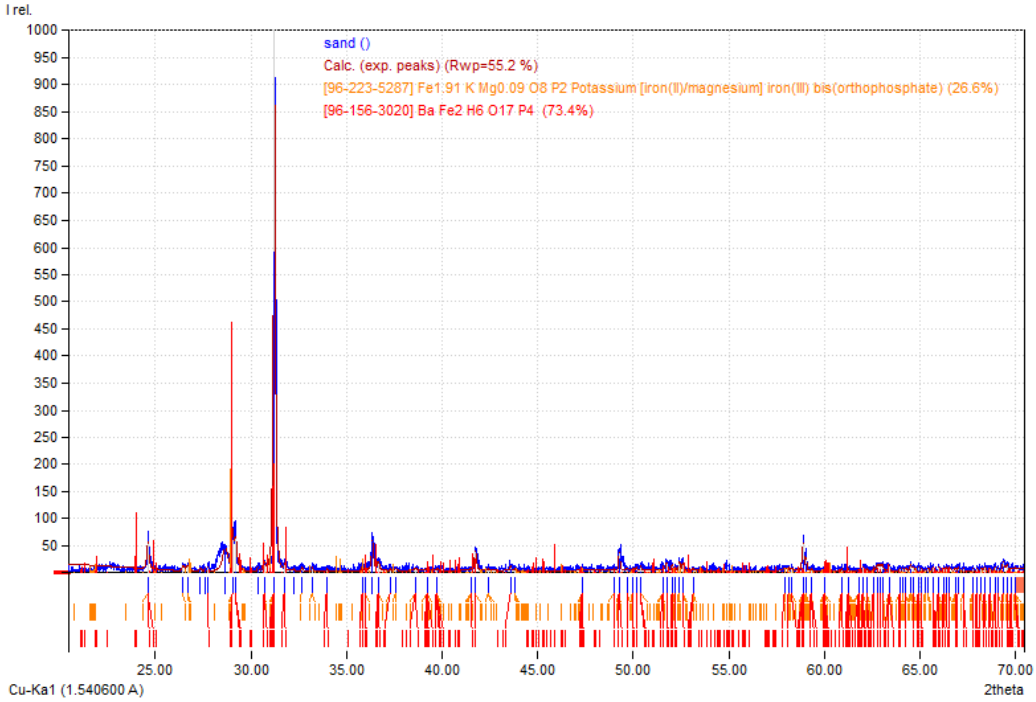
Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	28797	100.00%
Background radiation	9286	32.25%
Diffraction peaks	19511	67.75%
Peak area belonging to selected phases	8412	29.21%
Peak area of phase A (Potassium [iron(II)/magnesium] iron(III) bis(orthophosphate))	*2363*	*8.20%*
Peak area of phase B (Ba Fe2 H6 O17 P4)	*6050*	*21.01%*
Unidentified peak area	11098	38.54%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	235	100.00%
Peak intensity belonging to selected phases	217	92.39%
Unidentified peak intensity	18	7.61%

Diffraction Pattern Graphics



2. Hasil metode XRD untuk sampel titik 2

Match! Phase Analysis Report

Sample: sand ()

Sample Data

File name	titik#2.RAW
File path	C:/Program Files/Match3/geofisika/titik#2
Data collected	Jan 25, 2024 16:11:26
Data range	20.130º - 70.130º
Original data range	20.000º - 70.000º
Number of points	2501
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	No
2theta correction	0.13º
Radiation	X-rays
Wavelength	1.540600 Å

Index	***Amount (%)***	***Name***	***Formula sum***
A	34.4	Magnetite	Fe3 O4
6		Ferrocolumbite	Ca0.001 Fe0.747 Mn0.215 Nb1.894 O6 Sc0.003 Sn0.001 Ta0.094 Ti0.027 W0.003
8		*Unidentified peak area*	

Amount (weight %)

33.5%
32.8%
27.8%(*)

Ta	3.2%
Mn	2.2%
Ti	0.2%
W	0.1%
Sc	0.0%
Sn	0.0%
Ca	0.0%
*LE (sum)	27.8%

Details of identified phases

A: Magnetite (34.4 %)*

Formula sum	Fe3 O4
Entry number	96-900-2318
Figure-of-Merit (FoM)	0.699860*
Total number of peaks	36
Peaks in range	11
Peaks matched	8
Intensity scale factor	0.16
2theta correction	0.073°
Space group	F d -3 m
Crystal system	Cubic
Unit cell	a= 8.3837 Å
I/Ic	5.65
Calc. density	5.220 g/cm³
Reference	Haavik C., Stolen S., Fjellvag H., Hanfland M., Hausermann D., "Equation of state of magnetite and its high-pressure modification:Thermodynamics of the Fe-O system at high pressureSample at P = 1.4 GPa", American Mineralogist **85**, 514-523 (2000)

B: Ferrocolumbite (65.6 %)*

Formula sum	Ca0.001 Fe0.747 Mn0.215 Nb1.894 O6 Sc0.003 Sn0.001 Ta0.094 Ti0.027 W0.003
Entry number	96-900-7253
Figure-of-Merit (FoM)	0.720608*
Total number of peaks	475
Peaks in range	80
Peaks matched	41
Intensity scale factor	0.38
2theta correction	0.008°
Space group	P b c n
Crystal system	orthorhombic
Unit cell	a= 14.3191 Å b= 5.7482 Å c= 5.0713 Å
I/Ic	6.95
Calc. density	5.484 g/cm³
Reference	Tarantino S C, Zema M, Pistorino M, Domeneghetti M C, "High-temperature X-ray investigation of natural columbitesNote: sample BRA3 at T = 300 CLocality: San Jose de Safira, Minas Gerais, Brazil", Physics and Chemistry of Minerals **30**, 590-598 (2003)

(*)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Candidates

Formula	*Entry No.*	*FoM*
Cu2 Fe2 Ge4 O13	96-210-2753	0.6602
Cu2 Fe2 Ge4 O13	96-210-2754	0.6597

	Cu2 Fe2 Ge4 O13	96-210-2752	0.6550
	Cu2 Fe2 Ge4 O13	96-210-2751	0.6536
	Cu2 Fe2 Ge4 O13	96-210-2749	0.6464
	Cu2 Fe2 Ge4 O13	96-210-2750	0.6464
Cu2 Fe2 (Ge4 O13)	Cu2 Fe2 Ge4 O13	96-153-2854	0.6456
	Cu2 Fe2 Ge4 O13	96-210-2755	0.6426
	Cu2 Fe2 Ge4 O13	96-210-2756	0.6411
iron tungsten nitride	Fe3 N W3	96-200-6776	0.6137
Y Fe (Ge2 O7)	Fe Ge2 O7 Y	96-400-2474	0.6125

Search-Match

Settings

Reference database used	COD-Inorg 2023.12.05
Automatic zeropoint adaptation	Yes
Downgrade entries with low scaling factors	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	0
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Selection Criteria

Elements:

Elements that must be present: Fe

Elements that may be present: All elements not mentioned above

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0 (peak height)*	*Counts (peak area)*	*FWHM*	*Matched*
1	21.67	4.0977	9.68	4.20	0.1600	
2	21.89	4.0571	13.06	1.42	0.0400	
3	22.09	4.0208	17.72	5.77	0.1200	
4	22.27	3.9887	15.98	20.81	0.4800	
5	22.41	3.9641	4.54	2.46	0.2000	
6	23.23	3.8260	7.41	2.41	0.1200	
7	24.09	3.6913	91.76	39.85	0.1600	B
8	24.45	3.6378	4.69	1.02	0.0800	
9	24.79	3.5886	51.96	16.92	0.1200	B
10	25.07	3.5492	3.57	1.55	0.1600	
11	26.05	3.4178	27.40	11.90	0.1600	
12	26.59	3.3496	9.99	2.17	0.0800	B
13	26.97	3.3033	5.54	0.60	0.0400	
14	27.21	3.2747	5.56	1.81	0.1200	
15	27.95	3.1897	90.80	78.86	0.3200	
16	28.57	3.1218	22.57	9.80	0.1600	
17	30.09	2.9675	1000.00	325.70	0.1200	A,B
18	30.53	2.9257	27.92	27.28	0.3600	
	30.97	2.8852	38.71	21.01	0.2000	B
	31.43	2.8440	6.09	0.66	0.0400	
	31.99	2.7955	4.19	0.45	0.0400	
	32.73	2.7339	3.32	0.36	0.0400	
	32.87	2.7226	3.25	0.35	0.0400	
	33.47	2.6752	6.16	0.67	0.0400	B

25	35.23	2.5454	9.02	0.98	0.0400	B
26	35.37	2.5357	11.26	7.33	0.2400	A,B
27	35.91	2.4988	31.21	23.72	0.2800	B
28	36.27	2.4748	4.01	1.31	0.1200	B
29	36.95	2.4308	6.51	2.12	0.1200	A
30	40.49	2.2261	6.29	0.68	0.0400	B
31	42.07	2.1461	6.90	0.75	0.0400	
32	42.23	2.1383	5.07	0.55	0.0400	
33	43.07	2.0985	3.95	0.86	0.0800	A,B
34	45.03	2.0116	22.35	7.28	0.1200	B
35	46.93	1.9345	4.91	1.60	0.1200	
36	47.15	1.9260	4.76	1.03	0.0800	A,B
37	48.75	1.8665	7.18	0.78	0.0400	
38	50.11	1.8189	14.00	6.08	0.1600	
39	51.15	1.7844	10.07	3.28	0.1200	B
40	51.37	1.7772	8.43	0.92	0.0400	B
41	51.51	1.7727	9.41	1.02	0.0400	
42	51.65	1.7683	8.91	4.84	0.2000	B
43	52.57	1.7395	4.42	0.48	0.0400	B
44	52.71	1.7352	4.29	0.47	0.0400	B
45	54.87	1.6719	8.02	2.61	0.1200	B
46	57.05	1.6131	40.97	13.34	0.1200	A,B
47	57.23	1.6084	17.08	5.56	0.1200	
48	57.39	1.6043	4.12	0.89	0.0800	B
49	60.99	1.5179	6.95	1.51	0.0800	B
50	61.15	1.5144	3.42	0.74	0.0800	
51	62.57	1.4834	8.79	0.95	0.0400	A,B
52	62.85	1.4774	3.80	1.24	0.1200	B
53	64.09	1.4518	6.91	2.25	0.1200	B
54	64.35	1.4466	4.52	0.98	0.0800	
55	66.73	1.4006	13.79	4.49	0.1200	A,B

Integrated Profile Areas

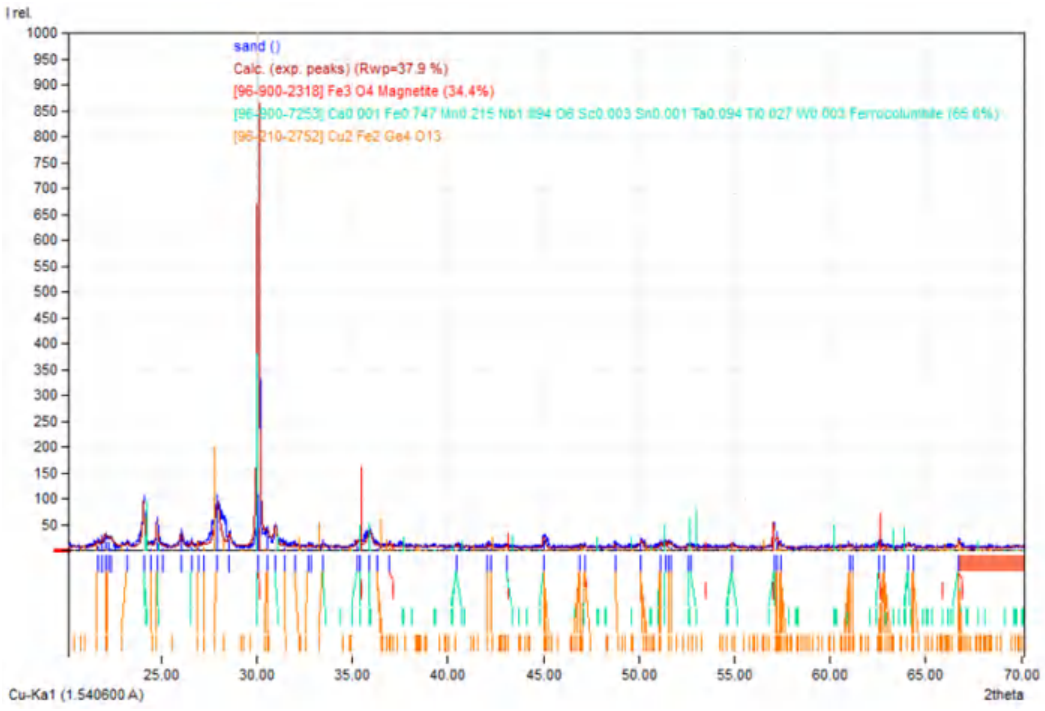
Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	87096	100.00%
Background radiation	42105	48.34%
Diffraction peaks	44991	51.66%
Peak area belonging to selected phases	10285	11.81%
Peak area of phase A (Magnetite)	*2210*	*2.54%*
Peak area of phase B (Ferrocolumbite)	*8075*	*9.27%*
Unidentified peak area	34706	39.85%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	679	100.00%
Peak intensity belonging to selected phases	638	94.07%
Unidentified peak intensity	40	5.93%

Diffraction Pattern Graphics



3. **Hasil metode XRD untuk sampel titik 3**

Match! Phase Analysis Report

Sample: sand ()

Sample Data

File name	titik#3.RAW
File path	C:/Program Files/Match3/geofisika/titik#3
Data collected	Jan 25, 2024 16:11:26
Data range	20.000º - 70.000º
Original data range	20.000º - 70.000º
Number of points	2501
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
Radiation	X-rays
Wavelength	1.540600 Å

dex	*Amount (%)*	*Name*	*Formula sum*
A	12.3	Magnetite	Fe2.719 O4 Si0.289
	45.9	Magnesium oxide Periclase	Mg O
	5.7	Hexaferrum	Fe0.69 Ir0.05 Ni0.02 Os0.18 Ru0.06
	17.7	Hematite	Fe2 O3
	18.4	Copper	Cu
	46.8	*Unidentified peak area*	

Amount (weight %)

27.7%

O	*27.0%(*)*
Fe	23.1%
Cu	18.4%
Os	2.2%
Ir	0.6%
Si	0.4%
Ru	0.4%
Ni	0.1%
**LE (sum)*	*27.0%*

Details of identified phases

A: Magnetite (12.3 %)*

Formula sum	Fe2.719 O4 Si0.289
Entry number	96-900-6923
Figure-of-Merit (FoM)	0.655044*
Total number of peaks	36
Peaks in range	10
Peaks matched	6
Intensity scale factor	0.30
2theta correction	-0.026°
Space group	F d -3 m
Crystal system	Cubic
Unit cell	a= 8.3740 Å
I/Ic	5.28
Calc. density	5.067 g/cm³
Reference	Yamanaka T., Shimazu H., Ota K., "Electric conductivity of Fe2SiO4-Fe3O4 spinel solid solutionsSample: Fe(3-x)SixO4, x = 0.288, synthesized at 1200 C, 10 GPa", Physics and Chemistry of Minerals **28**, 110-118 (2001)

B: Magnesium oxide Periclase (45.9 %)*

Formula sum	Mg O
Entry number	96-101-1119
Figure-of-Merit (FoM)	0.752039*
Total number of peaks	10
Peaks in range	3
Peaks matched	2
Intensity scale factor	0.69
2theta correction	0.005°
Space group	F m -3 m
Crystal system	Cubic
Unit cell	a= 4.2000 Å
I/Ic	3.22
Meas. density	3.560 g/cm³
Calc. density	3.613 g/cm³
Reference	Schiebold E, "Crystal Structure", Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik,Kristallchemie (-144,1977) **56**, 430-430 (1927)

C: Hexaferrum (5.7 %)*

Formula sum	Fe0.69 Ir0.05 Ni0.02 Os0.18 Ru0.06
Entry number	96-901-7842
lerit (FoM)	0.731130*
er of peaks	18
nge	4
:hed	3
ale factor	0.37
ection	-0.021°

Space group	P 63/m m c
Crystal system	Hexagonal
Unit cell	a= 2.5910 Å c= 4.1680 Å
I/Ic	13.70
Calc. density	12.283 g/cm³
Reference	Mochalov A. G., Dmitrenko G. G., Rudashevsky N. S., Zhernovsky I. V., Boldyreva M. M., "Hexaferrum (Fe,Ru),(Fe,Os),(Fe,Ir) - a new mineralNote: sample 117-8", Zapiski Vserossijskogo Mineralogicheskogo Obshchestva **127**, 41-51 (1998)

D: Hematite (17.7 %)*

Formula sum	Fe2 O3
Entry number	96-901-5504
Figure-of-Merit (FoM)	0.703120*
Total number of peaks	75
Peaks in range	14
Peaks matched	10
Intensity scale factor	0.31
2theta correction	0.029°
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 5.0020 Å c= 13.6202 Å
I/Ic	3.73
Calc. density	5.391 g/cm³
Reference	Finger L. W., Hazen R. M., "Crystal structure and isothermal compression of Fe2O3, Cr2O3, and V2O3 to 50 kbarsNote: P = 52.4 kbar", Journal of Applied Physics **51**, 5362-5367 (1980)

E: Copper (18.4 %)*

Formula sum	Cu
Entry number	96-901-3021
Figure-of-Merit (FoM)	0.733142*
Total number of peaks	8
Peaks in range	2
Peaks matched	2
Intensity scale factor	1.01
2theta correction	0.017°
Space group	F m -3 m
Crystal system	Cubic
Unit cell	a= 3.6670 Å
I/Ic	11.74
Calc. density	8.560 g/cm³
Reference	Suh I.-K., Ohta H., Waseda Y., "High-temperature thermal expansion of six metallic elements measuredby dilatation method and X-ray diffractionSample: at T = 1076 K", Journal of Materials Science **23**, 757-760 (1988)

(*)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Candidates

Formula	*Entry No.*	*FoM*
Cu0.8 Fe0.2	96-152-4702	0.7270
Ag16 As4 Fe0.526 Hg0.474 S15	96-901-5731	0.7255

.2)

Fluorarrojadite-(KFe)	Al Ca0.84 F2 Fe10.52 K0.83 Mg3.48 Na3.106 O48 P11.74 Pb0.17 Sr0.16	96-901-5723	0.7162
Barium diiron tetraoxide	Ba Fe2 O4	96-200-2359	0.7009
Franklinite	Fe2 O4 Zn	96-900-6903	0.7007
K Na5 Ca (Fe10 Mn3) Al F2 (P O4)12	Al Ca F2 Fe10 K Mn3 Na5 O48 P12	96-152-4952	0.7005
(Fe0.75 Pd0.25)	Fe0.75 Pd0.25	96-152-3351	0.6983
Arrojadite-(KFe)	Al Ca F2 Fe14 K Na4 O48 P12	96-900-0830	0.6954
Arrojadite-(KNa)	Al Ba0.06 Ca0.23 Fe11.69 K0.68 Mg1.85 Na4.459 O50 P12 Sr0.23	96-901-5152	0.6919
potassium iron germanate	Fe Ge K O4	96-200-8723	0.6832
ferric perchlorate nonahydrate	Cl3 Fe H18 O21	96-224-0190	0.6813
hexaaquairon(III) tris(perchlorate) trihydrate	Cl3 Fe H18 O21	96-220-8606	0.6804
	Bi3 Fe Mo2 O12	96-723-2466	0.6803
Fluorarrojadite-(KFe)	Al Ca1.168 F2 Fe12.26 K0.908 Mg2.52 Na3.152 O48 P11.916	96-901-5467	0.6775
Grandaite	Al0.68 As1.77 Ba0.079 Ca0.452 Fe0.14 H Mg0.13 Mn0.12 O9 Sr1.469 V0.23	96-901-7668	0.6775
Bi5.789 Nb10.01 Fe0.99 O35.492	Bi5.789 Fe0.99 Nb10.01 O35.492	96-152-8540	0.6747
Diopside	Al0.27 Ca0.52 Fe0.24 Mg0.66 Mn0.01 Na0.29 O6 Si2 Ti0.01	96-900-1338	0.6671
	Fe2 O3	96-152-8613	0.6670
	C0 F8 Fe2 N6 O8 P2	96-411-4284	0.6661
Diopside	Al0.029 Ca0.509 Cr0.223 Fe0.011 Mg0.488 Mn0.001 Na0.491 O6 Si1.99 Ti0.001V0.257	96-900-2723	0.6641
Diopside	Al0.035 Ca0.51 Cr0.247 Fe0.007 Mg0.484 Mn0.001 Na0.49 O6 Si1.982 V0.244	96-900-2722	0.6637
Diopside	Al0.22 Ca0.61 Fe0.2 Mg0.72 Na0.25 O6 Si2	96-900-1336	0.6635
Diopside	Al0.323 Ca0.661 Cr0.005 Fe0.206 Mg0.771 Mn0.001 Na0.153 O6 Si1.851 Ti0.029	96-900-5010	0.6630
Omphacite	Al0.51 Ca0.5 Fe0.06 Mg0.46 Na0.5 O6 Si1.97	96-901-1810	0.6614
(Na.118 Ca.553 Mg1.087 Fe.125 Fe.025 Al.119) Si1.973 O6	Al0.119 Ca0.553 Fe0.15 Mg1.087 Na0.118 O6 Si1.973	96-153-1794	0.6604
Diopside	Al0.42 Ca0.646 Fe0.271 Mg0.69 Mn0.003 Na0.143 O6 Si1.783 Ti0.044	96-900-4997	0.6600
Diopside	Ca0.58 Fe0.5 Mg0.5 Na0.42 O6 Si2	96-901-4599	0.6600
(Mg0.89 Fe0.11) Al2 (P O4)2 (O H)2	Al2 Fe0.11 H2 Mg0.89 O10 P2	96-154-2135	0.6598
cium magnesium iron titanium te * (Augite)	Al0.34 Ca0.6 Fe0.2 Mg0.9 Na0.1 O6 Si1.82	96-100-0036	0.6587
)2Fe0.01Al0.99Si2.99O8 (albite)	Al0.99 Fe0.01 K0.01 Na1.02 O8 Si2.99	96-155-7000	0.6582
	Al0.25 Ca0.645 Cr0.044 Fe0.112 Mg0.957 Mn0.002 Na0.094 O6	96-900-5235	0.6580

Labyrinthite	Si1.888 Ti0.008 Ca12 Ce0.102 Cl2.68 F0.68 Fe2.19 H11.56 K1.452 Mn0.81 Na34.53 O151.54 Si51.2Sr0.735 Ti0.52 Zr6	96-901-2646	0.6565
Fe Zn Sb	Fe Sb Zn	96-152-0977	0.6564
Iron	Fe	96-901-4477	0.6560
Iron	Fe	96-901-4712	0.6560
Iron	Fe	96-901-5072	0.6560
Diopside	Al0.444 Ca0.637 Cr0.001 Fe0.29 Mg0.647 Mn0.004 Na0.159 O6 Si1.772 Ti0.046	96-900-4998	0.6555
Lazulite	Al2 Fe0.134 H2 Mg0.866 O10 P2	96-900-9305	0.6552
Franklinite	Fe2 O4 Zn	96-900-6902	0.6549
(B5 Er8 Fe70 Si2)0.024	B0.118 Er0.188 Fe1.648 Si0.048	96-151-1038	0.6535
Pigeonite	Al0.02 Ca0.121 Fe1.008 Mg0.871 O6 Si1.98	96-901-3710	0.6528
Diopside	Al0.426 Ca0.631 Fe0.295 Mg0.662 Mn0.004 Na0.163 O6 Si1.777 Ti0.042	96-900-5000	0.6526
Tribarium diiron(III) digallium dialuminium oxide	Al2 Ba3 Fe2 Ga2 O12	96-200-2554	0.6516
Diopside	Al0.32 Ca0.55 Fe0.15 Mg0.65 Na0.3 O6 Si2 Ti0.01	96-900-1339	0.6506
	Fe3 N1.235	96-152-5732	0.6505
Silver iron (0.3/0.7)	Ag0.3 Fe0.7	96-150-9089	0.6504
Katayamalite	Ca7 F0.24 Fe0.05 H1.76 K0.89 Li3 Na0.11 O37.76 Si12 Ti1.95	96-901-2100	0.6494
Ca.818 Mg.792 Fe.183 Fe.086 Al.151 Al.269 Si1.731 O6	Al0.42 Ca0.818 Fe0.269 Mg0.792 O6 Si1.731	96-152-6738	0.6493
Enstatite	Al0.03 Fe0.15 Mg1.82 O6 Si1.97	96-901-0889	0.6490
Aegirine	Ca0.25 Fe Na0.75 O6 Si2	96-900-5437	0.6487
Enstatite	Al0.03 Fe0.15 Mg1.82 O6 Si1.97	96-901-0897	0.6477
Iron cobalt sulfide	Co Fe S2	96-101-0434	0.6470

and 178 others...

Search-Match

Settings

Reference database used	COD-Inorg 2023.12.05
Automatic zeropoint adaptation	Yes
Downgrade entries with low scaling factors	Yes
Minimum figure-of-merit (FoM)	0.60
low for peak corr.	0.30 deg.
el. int. for peak corr.	0
influence 2theta	0.50
influence intensities	0.50
multiple/single phase(s)	0.50

Selection Criteria

Elements:

Elements that must be present: Fe

Elements that may be present: All elements not mentioned above

Peak List

No.	*2theta [°]*	*d [Å]*	*I/I0 (peak height)*	*Counts (peak area)*	*FWHM*	*Matched*
1	20.12	4.4098	52.36	2.02	0.0647	
2	20.26	4.3796	1.62	0.10	0.1033	
3	20.40	4.3499	36.97	2.28	0.1033	
4	20.48	4.3331	29.80	1.84	0.1033	
5	20.92	4.2429	110.96	5.30	0.0800	
6	21.14	4.1993	28.10	1.34	0.0800	
7	21.34	4.1604	35.13	1.68	0.0800	
8	21.66	4.0996	5.64	0.27	0.0800	
9	22.02	4.0334	218.72	13.69	0.1049	
10	22.28	3.9869	9.34	0.45	0.0800	
11	23.28	3.8179	8.39	0.22	0.0441	
12	23.90	3.7202	53.78	6.67	0.2081	
13	24.10	3.6898	10.90	2.41	0.3705	
14	24.24	3.6688	12.04	1.55	0.2163	D
15	26.10	3.4114	19.43	1.48	0.1275	
16	26.88	3.3142	15.29	0.45	0.0489	
17	27.48	3.2431	34.56	8.00	0.3880	
18	27.58	3.2316	82.74	5.92	0.1200	
19	27.92	3.1930	865.01	73.05	0.1416	
20	28.14	3.1686	78.54	4.22	0.0900	
21	28.52	3.1272	19.25	1.33	0.1160	
22	28.70	3.1080	17.45	0.45	0.0431	
23	29.66	3.0095	14.67	0.46	0.0523	
24	29.88	2.9879	91.19	6.15	0.1131	
25	30.12	2.9646	71.51	5.71	0.1339	A
26	30.28	2.9493	84.10	5.45	0.1087	
27	30.56	2.9229	141.61	10.14	0.1200	
28	30.76	2.9044	15.10	2.94	0.3268	
29	31.04	2.8788	20.82	2.22	0.1786	
30	31.34	2.8519	15.68	1.14	0.1219	
31	31.62	2.8273	15.58	0.54	0.0580	
32	31.84	2.8083	67.29	4.74	0.1180	
33	32.90	2.7202	31.03	2.46	0.1331	
34	33.38	2.6822	118.23	20.07	0.2846	D
35	33.88	2.6437	42.89	2.05	0.0800	
36	35.22	2.5461	133.18	9.53	0.1200	
37	35.30	2.5406	49.10	1.51	0.0517	
38	35.60	2.5198	108.95	10.40	0.1600	A
39	35.80	2.5062	137.64	14.46	0.1761	D
40	35.96	2.4954	70.42	25.21	0.6000	
41	36.10	2.4861	162.28	7.70	0.0795	
42	40.02	2.2511	141.83	5.46	0.0645	
	40.12	2.2457	54.12	2.29	0.0710	C
	41.10	2.1944	72.46	11.56	0.2674	D
	42.64	2.1187	1000.00	65.66	0.1101	E
	43.04	2.0999	36.94	20.27	0.9200	B
	43.16	2.0943	113.19	8.10	0.1200	A
	43.30	2.0879	98.63	11.77	0.2000	
	43.44	2.0815	49.24	3.53	0.1200	C

50	45.92	1.9747	466.60	19.33	0.0694	C
51	46.46	1.9530	17.01	0.54	0.0527	
52	46.86	1.9372	9.52	0.49	0.0855	
53	47.06	1.9295	7.94	0.22	0.0466	A
54	49.00	1.8575	16.84	0.80	0.0794	
55	49.42	1.8427	13.58	1.24	0.1529	
56	49.70	1.8330	54.66	7.03	0.2154	E
57	49.78	1.8302	44.52	13.81	0.5200	D
58	49.94	1.8247	28.48	2.28	0.1342	
59	50.06	1.8206	10.82	0.52	0.0799	
60	50.38	1.8098	18.54	0.81	0.0732	
61	50.60	1.8025	277.85	15.03	0.0907	
62	50.74	1.7978	123.68	5.19	0.0703	
63	52.00	1.7572	139.31	7.24	0.0872	
64	54.38	1.6858	49.03	15.06	0.5149	
65	54.50	1.6823	46.10	3.30	0.1200	D
66	56.72	1.6217	290.13	13.83	0.0799	D
67	56.88	1.6175	130.37	5.76	0.0741	
68	57.20	1.6092	102.36	10.67	0.1748	A
69	58.62	1.5735	15.16	2.25	0.2490	
70	59.72	1.5472	21.91	1.05	0.0800	
71	62.48	1.4853	277.55	19.87	0.1200	B
72	62.66	1.4814	164.10	16.42	0.1677	A
73	62.94	1.4755	56.97	9.24	0.2720	D
74	63.62	1.4614	171.53	8.84	0.0863	
75	63.76	1.4585	53.13	3.99	0.1260	
76	63.94	1.4548	24.23	2.36	0.1631	
77	64.78	1.4380	19.65	0.62	0.0531	D
78	66.42	1.4064	119.76	7.38	0.1033	
79	66.60	1.4030	58.24	2.59	0.0746	D

Integrated Profile Areas

Based on calculated profile

Profile area	***Counts***	***Amount***
Overall diffraction profile	42975	100.00%
Background radiation	13339	31.04%
Diffraction peaks	29636	68.96%
Peak area belonging to selected phases	9542	22.20%
Peak area of phase A (Magnetite)	*1435*	*3.34%*
Peak area of phase B (Magnesium oxide Periclase)	*2037*	*4.74%*
Peak area of phase C (Hexaferrum)	*1072*	*2.50%*
Peak area of phase D (Hematite)	*2384*	*5.55%*
Peak area of phase E (Copper)	*2614*	*6.08%*
Unidentified peak area	20094	46.76%

Peak Residuals

Peak data	***Counts***	***Amount***
Overall peak intensity	594	100.00%
Peak intensity belonging to selected phases	557	93.81%
Unidentified peak intensity	37	6.19%

Diffraction Pattern Graphics