

## DAFTAR PUSTAKA

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## Foto sampel

### 1. Sampel I



Koordinat : 5°13'43,30" LS - 119°39'42,95" BT  
Warna segar : Hitam keabu-abuan  
Warna lapuk : Hitam kelam  
Tekstur : Keras  
Kandungan mineral : *Diopside, Enstatite, Pigeoite* dan *Albite*  
Senyawa kimia :  $\text{MgCaSi}_2\text{O}_6$ ,  $\text{MgSiO}_3$ ,  $(\text{Ca},\text{Mg},\text{Fe})(\text{Mg},\text{Fe})\text{Si}_2\text{O}_6$ ,  
 $\text{NaAlSi}_3\text{O}_8$

### 2. Sampel II



Koordinat : 5°13'42,65" LS - 119°39'43,89" BT

Warna segar : Hitam keabu-abuan  
Warna lapuk : Hitam kelam  
Tekstur : Keras  
Kandungan mineral : *Bytownite, Diopside* dan *Albite*  
Senyawa kimia :  $(Ca,Na)[Al(Al,Si)Si_2O_8]$ ,  $MgCaSi_2O_6$ ,  $NaAlSi_3O_8$

### 3. Sampel III



Koordinat :  $5^{\circ}13'43,19''$  LS -  $119^{\circ}39'45,12''$  BT  
Warna segar : Hitam keabu-abuan  
Warna lapuk : Hitam kelam  
Tekstur : Keras  
Kandungan mineral : *Pigeonite, Albite*, dan *Diopside*  
Senyawa kimia :  $(Ca,Mg,Fe)(Mg,Fe)Si_2O_6$ ,  $NaAlSi_3O_8$ ,  $MgCaSi_2O_6$

### 4. Sampel IV



Koordinat : 5°13'43,09" LS - 119°39'46,32" BT  
Warna segar : Hitam keabu-abuan  
Warna lapuk : Hitam kelam  
Tekstur : Keras  
Kandungan mineral : *Anorthite* dan *Pigeonite*  
Senyawa kimia :  $\text{CaAl}_2\text{Si}_2\text{O}_8, (\text{Ca},\text{Mg},\text{Fe})(\text{Mg},\text{Fe})\text{Si}_2\text{O}_6$

#### 5. Sampel V



Koordinat : 5°13'42,83" LS - 119°39'54,24" BT  
Warna segar : Hitam keabu-abuan  
Warna lapuk : Hitam kelam  
Tekstur : Keras  
Kandungan mineral : *Anorthite*, *Albite*, *Pigeonite* dan *Magnetite*  
Senyawa kimia :  $\text{CaAl}_2\text{Si}_2\text{O}_8, \text{NaAlSi}_3\text{O}_8, (\text{Ca},\text{Mg},\text{Fe})(\text{Mg},\text{Fe})\text{Si}_2\text{O}_6$   
 $\text{Fe}_3\text{O}_4$

6. Sampel VI



Koordinat : 5°13'44,23" LS - 119°39'54,77" BT

Warna segar : Hitam keabu-abuan

Warna lapuk : Hitam kelam

Tekstur : Keras

Kandungan mineral : *Albite, Pigeonite, Diopside* dan *Periclase*

Senyawa kimia :  $\text{NaAlSi}_3\text{O}_8$ ,  $(\text{Ca},\text{Mg},\text{Fe})(\text{Mg},\text{Fe})\text{Si}_2\text{O}_6$ ,  $\text{MgCaSi}_2\text{O}_6$ ,  
MgO



# Match! Phase Analysis Report

## Sample: batuan ()

**Sample Data**  
File name 1B#mhs#S1#2020.ORG  
File path D:/Data/ App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/1B#mhs#S1#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 20.090° - 65.090°  
Number of points 2251  
Step size 0.020  
Rietveld refinement converged  
N  
o Alpha2 subtracted  
N  
o  
Background subtr. Yes  
Data smoothed Yes  
2theta correction 0.09°  
Radiation X-rays  
Wavelength 1.540600 Å

## Matched Phases

Index	Amount (%)	Name	Formula sum
A	38.1	Diopside	Ca Mg O6 Si2
B	34.2	Pigeonite	Ca0.15 Mg1.85 O6 Si2
C	19.0	Enstatite	Al0.03 Fe0.15 Mg1.82 O6 Si1.97
D	8.8	Albite	Al Na O8 Si3

### A: Diopside (38.1 %)

Formula sum Ca Mg O6 Si2  
Entry number 96-900-0799  
Figure-of-Merit (FoM) 0.818698  
Total number of peaks 221  
Peaks in range 71  
Peaks matched 55  
Intensity scale factor 0.44  
Space group C 1 2/c 1  
Crystal system monoclinic  
Unit cell a= 9.6809 Å b= 8.8470 Å c= 5.2169 Å β= 105.570 °  
I/Icor 1.22  
Calc. density 3.342 g/cm<sup>3</sup>  
Reference Levien L., Prewitt C. T., "High-pressure structural study of diopside P = 23.6 kbar pyroxene", American Mineralogist **66**, 315-323 (1981)

### B: Pigeonite (34.2 %)

Formula sum Ca0.15 Mg1.85 O6 Si2  
Entry number 96-900-3110  
Figure-of-Merit (FoM) 0.792618  
Total number of peaks 417  
Peaks in range 128  
Peaks matched 86  
Intensity scale factor 0.35

Space group P 1 21/c 1  
Crystal system monoclinic  
Unit cell a= 9.5460 Å b= 8.7320 Å c= 5.1490 Å β= 108.120 °  
I/Icor 0.93  
Calc. density 3.306 g/cm<sup>3</sup>  
Reference Nestola F., Tribaudino M., Ballaran T. B., "High pressure behavior, transformation and crystal structure of synthetic iron-free pigeonite Sample: P = 2.6 GPa", *American Mineralogist* **89**, 189-196 (2004)

**C: Enstatite (19.0 %)**

Formula sum Al<sub>0.03</sub> Fe<sub>0.15</sub> Mg<sub>1.82</sub> O<sub>6</sub> Si<sub>1.97</sub>  
Entry number 96-901-0892  
Figure-of-Merit (FoM) 0.800148  
Total number of peaks 444  
Peaks in range 137  
Peaks matched 98  
Intensity scale factor 0.12  
Space group P b c a  
Crystal system orthorhombic  
Unit cell a= 18.4378 Å b= 8.9555 Å c= 5.2711 Å  
I/Icor 0.68  
Calc. density 3.125 g/cm<sup>3</sup>  
Reference Gatta G. D., Rinaldi R., Knight K. S., Molin G., Artioli G., "High temperature structural and thermoelastic behaviour of mantle orthopyroxene: an in situ neutron powder diffraction study Sample: T = 1,125 C", *Physics and Chemistry of Minerals* **34**, 185-200 (2007)

**D: Albite (8.8 %)**

Formula sum Al Na O<sub>8</sub> Si<sub>3</sub>  
Entry number 96-900-0586  
Figure-of-Merit (FoM) 0.822724  
Total number of peaks 250  
Peaks in range 219  
Peaks matched 165  
Intensity scale factor 0.07  
Space group C -1  
Crystal system triclinic (anorthic)  
Unit cell a= 8.2420 Å b= 12.8410 Å c= 7.1760 Å α= 93.700° β= 116.300° γ= 87.600°  
I/Icor 0.82  
Calc. density 2.564 g/cm<sup>3</sup>  
Reference Winter J. K., Ghose S., Okamura F. P., "A high-temperature study of the thermal expansion and the anisotropy of the sodium atom in low albite T = 750 deg C Note: this sample of feldspar is from Tiburon, Marin County, California, USA", *American Mineralogist* **62**, 921-931 (1977)

## Candidates

<b>Name</b>	<b>Formula</b>	<b>Entry No.</b>	<b>FoM</b>
Barium molybdenum nitride	Ba3 Mo N4	96-700-9096	0.7872
Dithulium barium nickel oxide	Ba Ni O5 Tm2	96-100-6062	0.7871
cerium ytterbium sulfide	Ce3 S9 Yb3	96-400-1293	0.7871
	Bi Cs5 P4 Se12	96-410-3944	0.7871
	Ga0.5 Gd5 Ge3.5	96-411-4467	0.7871
holmium zinc antimonide (6/1/14)	Ho6 Sb14 Zn1.13	96-430-5533	0.7871
	D2 K O4 P	96-810-0990	0.7871
Diytterbium barium nickel oxide	Ba Ni O5 Yb2	96-100-6063	0.7870
Cs2Cu7(P2O7)4*6CsCl	Cl6 Cs 8 Cu7 O28 P8	96-431-3070	0.7869
Co5BP3O14	B Co5 O14 P3	96-432-3980	0.7869
Diopside	Ca0.5 Cr0.5 Mg0.5 Na0.5 O6 Si2	96-900-5706	0.7869
Pentacadmium tecto-divanado(III)vanado(IV)hexaphosphate	Cd5 O25 P6 V3	96-100-1569	0.7868
	Cu3 In2 O18 Se6	96-430-2744	0.7868
Sapphirine	Ga3.557 Ge1.225 Mg2.218 O10	96-900-5377	0.7868
Whitlockite	Ca9.5 Mg O28 P7	96-901-2138	0.7868
	Ga3.25 La12 Sb24.02	96-810-3053	0.7867
Normandite	Ca0.936 F Mn0.784 Na1.28 Nb0.124 O8 Si2 Ti0.876	96-900-4559	0.7867
Barium titanium niobium oxide (1/3/4/17)	Ba Nb4 O17 Ti3	96-100-1354	0.7866
	Gd5 Ge2.5 Si1.5	96-400-0244	0.7866
	P Rb Se6	96-431-0932	0.7866
	Cs10 P8 Se20	96-431-5307	0.7865
Barytolamprophyllite	Al0.03 Ba0.88 Ca0.13 Fe0.35 K0.61 Mg0.05 Mn0.28 Na2.09 Nb0.01 O18 Si4 Sr0.33 Ti2.91	96-901-0663	0.7865
Clinocervantite	O2 Sb	96-901-2518	0.7865
	Ga5.5 La3 Nb0.5 O14	96-210-3503	0.7864
Disilver(I) tricobalt(II) hydrogenphosphate bis(phosphate)	Ag2 Co3 H O12 P3	96-223-0800	0.7864
	O18 Se5 Sr2 V3	96-431-7370	0.7864
	Au46.67 Ca14 Sn4.15	96-432-4524	0.7864
	B8 Ca6.6 Cd1.4 O20	96-810-3055	0.7864
Diopside	B0.022 Ca0.82 Mg0.846 Na0.168 O6 Si1.882 Ti0.272	96-900-5679	0.7864
Muckeite	Bi0.9 Cu Ni S3 Sb0.1	96-900-7732	0.7864
Qitianlingite	Fe1.345 Mn0.559 Nb1.691 O10 Sn0.016 Ta0.351 Ti0.102 W0.919	96-901-3116	0.7864
Donpeacorite	Al0.003 Ca0.024 Mg1.433 Mn0.541 O6 Si1.997 Ti0.002	96-900-3576	0.7862
Lithium caesium polyphosphate	Cs Li O6 P2	96-100-8337	0.7861
Sodium tribismuth tetraoxide diiodide	Bi3 I2 Na O4	96-101-0167	0.7860
Diopside	Al Ca Mg0.5 O6 Si1.5	96-900-5281	0.7860
Zinc silver catena-phosphate	Ag O9 P3 Zn	96-100-7093	0.7859
	Cd O12 Rb2 Si5	96-200-5336	0.7859
	Ga0.9 La2 O4.55 Ti0.1	96-210-4431	0.7858
\alpha-Zn4Sb3	Sb10 Zn13	96-411-3279	0.7858
Montbrayite	Au2 Te3	96-901-1583	0.7858
Icosa Cerium nonadeca Magnesium henocataconta Zinc	Ce20 Mg19 Zn81	96-201-6697	0.7856
	Cs2 Ga O10 P3	96-700-9289	0.7856
Diopside	B0.018 Ca0.916 Mg0.926 Na0.066 O6 Si1.96 Ti0.086	96-900-5678	0.7856
Balyakinite	Cu O3 Te	96-900-9911	0.7856
	Ba2 Cl7 Gd	96-400-1655	0.7855
Albite	Al Na O8 Si3	96-900-0705	0.7855
Diopside	Ca0.8 Mg1.2 O6 Si2	96-900-4954	0.7855
Enstatite	Mg O3 Si	96-900-6341	0.7855
Osmium selenide	Os Se2	96-591-0035	0.7854
Enstatite	Fe0.249 Mg0.751 O3 Si	96-900-1644	0.7854
Bearthite	Al Ca2 H O9 P2	96-901-2868	0.7854
	Br H4 Na9 O20 S4	96-210-0330	0.7853

and 153 others...

### Search-Match

#### Settings

Reference database used COD-Inorg  
REV81284 2013.04.15 Automatic zeropoint  
adaptation Yes  
Minimum figure-of-merit (FoM) 0.60  
Parameter/influence 2theta 0.50  
Parameter/influence intensities 0.50  
Parameter multiple/single phase(s) 0.50

### Peak List

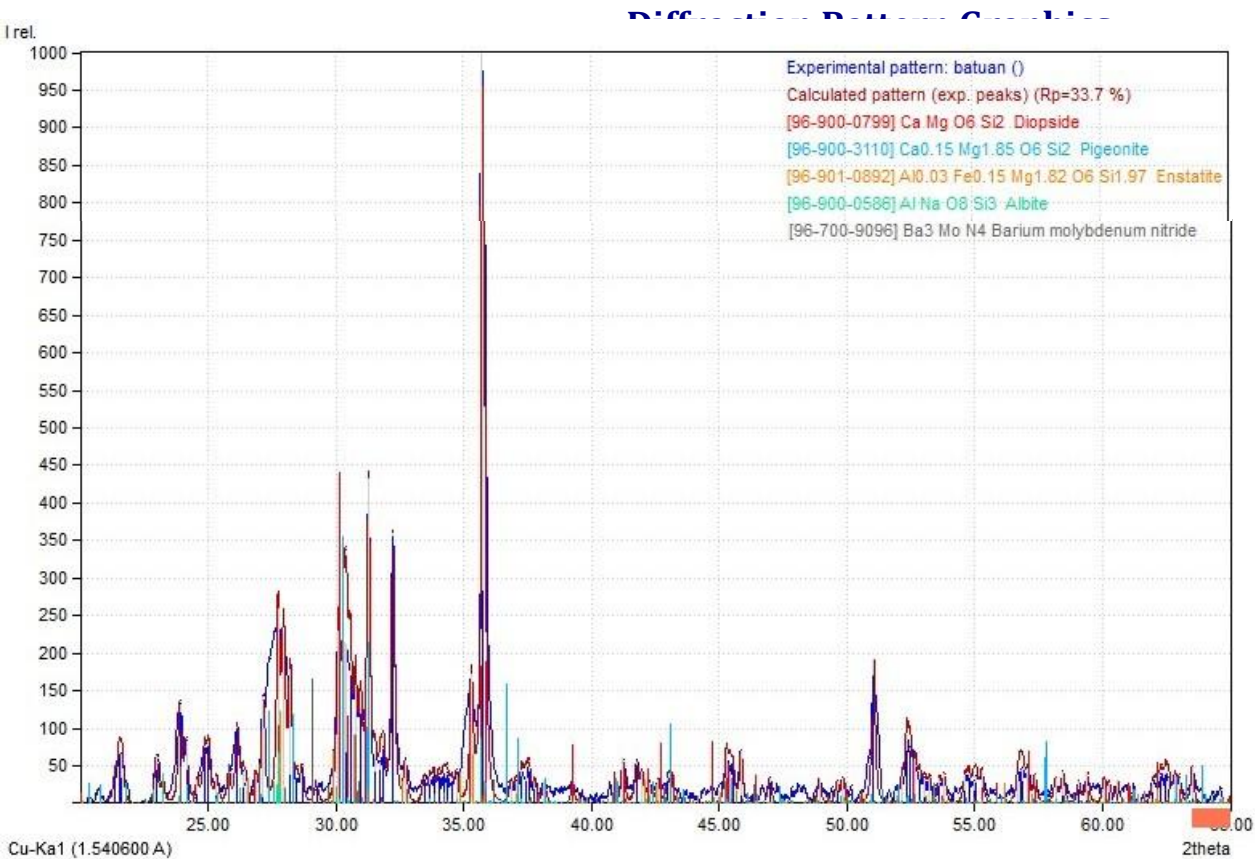
No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	21.35	4.1581	31.94	0.1600	
2	21.51	4.1276	62.54	0.1600	

3	21.63	4.1045	65.94	0.1600	C,D
4	22.98	3.8670	62.74	0.1600	D
5	23.24	3.8241	29.39	0.1600	D
6	23.90	3.7199	132.18	0.1600	D
7	24.15	3.6821	80.48	0.1600	C,D
8	24.58	3.6188	29.93	0.1600	A,B
9	24.87	3.5777	71.13	0.1600	
10	25.02	3.5567	74.95	0.1600	
11	25.34	3.5126	34.43	0.1600	B,D
12	25.81	3.4493	41.02	0.1600	D
13	26.14	3.4057	101.18	0.1600	C
14	26.36	3.3779	41.00	0.1600	D
15	26.49	3.3619	28.12	0.1600	C
16	26.89	3.3135	34.19	0.1600	A
17	27.16	3.2802	142.24	0.1600	B
18	27.74	3.2131	259.47	0.1600	A,C,D
19	27.96	3.1891	226.55	0.1600	C,D
20	28.22	3.1594	178.55	0.1600	B,D
21	28.48	3.1314	33.51	0.1600	
22	28.69	3.1095	46.30	0.1600	
23	29.24	3.0519	28.33	0.1600	B,C
24	30.11	2.9659	228.53	0.1600	A,C,D
25	30.31	2.9465	214.73	0.1600	B

26	30.41	2.9366	212.81	0.1600	A
27	30.57	2.9224	181.63	0.1600	D
28	30.77	2.9034	154.18	0.1600	C,D
29	30.97	2.8850	126.14	0.1600	B
30	31.28	2.8577	431.67	0.1600	A,B,C
31	31.53	2.8348	58.23	0.1600	C,D
32	31.74	2.8173	55.39	0.1600	A,D
33	31.87	2.8058	72.84	0.1600	D
34	32.24	2.7745	360.02	0.1600	B
35	32.73	2.7343	57.08	0.1600	B,C
36	33.45	2.6767	34.62	0.1600	D
37	33.68	2.6591	32.00	0.1600	D
38	33.83	2.6475	36.82	0.1600	
39	34.04	2.6317	37.09	0.1600	C
40	34.21	2.6188	35.85	0.1600	
41	34.35	2.6083	40.24	0.1600	C
42	34.53	2.5955	27.79	0.1600	
43	34.71	2.5824	38.24	0.1600	B,C,D
44	35.31	2.5400	170.94	0.1600	A,C,D
45	35.76	2.5087	1000.00	0.1600	A,B,C,D
46	36.86	2.4368	28.29	0.1600	B,C,D
47	37.06	2.4241	29.60	0.1600	B,C,D
48	37.27	2.4108	43.76	0.1600	D
49	37.42	2.4013	32.46	0.1600	B,D
50	37.56	2.3930	48.97	0.1600	C
51	37.78	2.3796	28.16	0.1600	A
52	38.15	2.3569	28.63	0.1600	B,C,D
53	39.27	2.2925	27.75	0.1600	A,B,C,D
54	41.23	2.1877	60.66	0.1600	A,B,C,D
55	41.77	2.1610	53.91	0.1600	B,D
56	41.98	2.1506	38.89	0.1600	C,D
57	42.27	2.1362	27.52	0.1600	A,B,C,D
58	42.61	2.1200	31.71	0.1600	A,B,C,D
59	43.00	2.1017	32.35	0.1600	D
60	43.13	2.0959	33.21	0.1600	A,B,C,D
61	45.28	2.0012	66.48	0.1600	A,B,C,D
62	45.42	1.9954	42.47	0.1600	A,B,D
63	45.53	1.9905	43.14	0.1600	
64	45.86	1.9769	69.26	0.1600	B,C,D
65	46.97	1.9329	33.82	0.1600	A,B,C,D
66	48.92	1.8605	32.92	0.1600	A,B,C,D
67	49.62	1.8359	29.22	0.1600	C,D
68	49.85	1.8278	32.16	0.1600	A,B,C,D
69	51.05	1.7877	190.60	0.1600	A,B,D
70	52.15	1.7525	29.90	0.1600	B,C,D
71	52.34	1.7467	90.26	0.1600	B
72	52.47	1.7424	74.39	0.1600	C,D
73	52.67	1.7363	53.38	0.1600	A,B,C,D
74	52.85	1.7309	37.58	0.1600	D
75	53.04	1.7251	32.15	0.1600	C,D
76	53.23	1.7195	33.50	0.1600	B,C
77	53.61	1.7081	32.26	0.1600	A,B,C,D
78	53.81	1.7024	38.69	0.1600	A,B,C,D
79	54.62	1.6791	36.76	0.1600	B,C,D
80	54.77	1.6747	38.53	0.1600	B,D
81	54.95	1.6695	28.99	0.1600	A,B,C,D
82	55.06	1.6666	34.14	0.1600	B,C
83	55.27	1.6607	43.35	0.1600	A,C,D
84	56.67	1.6229	29.49	0.1600	B,C,D
85	56.78	1.6201	43.83	0.1600	D
86	56.89	1.6172	44.90	0.1600	A,B,C,D
87	57.06	1.6128	41.39	0.1600	A,C,D
88	57.37	1.6049	36.60	0.1600	A,B,C,D
89	58.15	1.5851	32.86	0.1600	B,C,D
90	58.45	1.5778	41.78	0.1600	A,B,C,D
91	59.07	1.5627	29.14	0.1600	A,B,C,D
92	59.40	1.5547	41.57	0.1600	A,B,C,D
93	60.06	1.5393	31.13	0.1600	A,B,C,D
94	60.25	1.5349	27.46	0.1600	C,D
95	60.59	1.5270	29.89	0.1600	A,B,C,D
96	61.98	1.4961	29.26	0.1600	A,B,C,D
97	62.14	1.4925	33.73	0.1600	A,B,C
98	62.30	1.4892	37.68	0.1600	C,D
99	62.47	1.4855	41.10	0.1600	C,D
100	62.59	1.4829	34.04	0.1600	A,B,D
101	62.83	1.4778	35.21	0.1600	B,C,D
102	63.01	1.4741	33.35	0.1600	A,B,C,D
103	63.51	1.4637	48.90	0.1600	A,B,D

### Rietveld Refinement using FullProf

Calculation was not run or did not converge.



# Match! Phase Analysis Report

## Sample: tanah ()

**Sample Data**  
File name S1#2C#2020.ORG  
File path D:/Data/App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/S1#2C#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 19.910° - 64.910°  
Number of points 2251  
Step size 0.020  
Rietveld refinement  
converged No  
Alpha2 subtracted No  
Background subtr. Yes  
Data smoothed Yes  
2theta correction -0.09°  
Radiation X-rays  
Wavelength 1.540600 Å

## Matched Phases

Index	Amount (%)	Name	Formula sum
A	48.6	Bytownite	Al7.76 Ca3.44 Na0.56 O32 Si8.24
B	26.3	Diopside	Ca Mg O6 Si2
C	25.1	Albite	Al1.005 Na0.986 O8 Si2.995

### A: Bytownite (48.6 %)

Formula sum Al7.76 Ca3.44 Na0.56 O32 Si8.24  
Entry number 96-901-1202  
Figure-of-Merit (FoM) 0.857808  
Total number of peaks 500  
Peaks in range 469  
Peaks matched 284  
Intensity scale factor 0.40  
Space group P -1  
Crystal system triclinic (anorthic)  
Unit cell a= 8.1830 Å b= 12.8830 Å c= 14.1860 Å  $\alpha$ = 93.380°  $\beta$ = 115.870°  $\gamma$ = 90.820°  
I/Icor 0.60  
Calc. density 2.729 g/cm<sup>3</sup>  
Reference Facchinelli A., Bruno E., Chiari G., "The structure of bytownite quenched from 1723 K Locality: satellite dyke, Traversella stock, Sesia Lanzo zone, Western Alps, Italy Sample: BytQ, P-1 model", Acta Crystallographica, Section B **35(1)**, 34-42 (1979)

### B: Diopside (26.3 %)

Formula sum Ca Mg O6 Si2  
Entry number 96-100-0008  
Figure-of-Merit (FoM) 0.830997  
Total number of peaks 231  
Peaks in range 69  
Peaks matched 60  
Intensity scale factor 0.33  
Space group C 1 2/c 1  
Crystal system monoclinic  
Unit cell a= 9.7397 Å b= 8.9174 Å c= 5.2503 Å  $\beta$ = 105.866°

I/Icor 1.29  
 Calc. density 3.278 g/cm<sup>3</sup>  
 Reference Thompson R. M., Downs R. T., "The crystal structure of diopside at pressure to 10 GPa Locality: DeKalb, New York Sample: P = 1 atm", American Mineralogist **93**, 177-186 (2008)

**C: Albite (25.1 %)**

Formula sum Al1.005 Na0.986 O8 Si2.995  
 Entry number 96-900-0784  
 Figure-of-Merit (FoM) 0.875760  
 Total number of peaks 250  
 Peaks in range 208  
 Peaks matched 167  
 Intensity scale factor 0.21  
 Space group C -1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 8.1420 Å b= 12.7850 Å c= 7.1590 Å α= 94.190° β= 116.610 ° γ= 87.680 °  
 I/Icor 0.84  
 Calc. density 2.616 g/cm<sup>3</sup>  
 Reference Harlow G. E., Brown G. E., "Low albite: An X-Ray and neutron diffraction study Sample: X-ray single Na atom Note: this sample of feldspar is from Amelia, Virginia", American Mineralogist **65**, 986-995 (1980)

## Candidates

Name	Formula	Entry No.	FoM
1,10-octachlorophenanthroline	C12 Cl8 N2	96-432-3462	0.7989
Molybdenum tellurium oxide (5/1/16)	Mo5 O16 Te	96-100-8015	0.7976
Tellurium molybdenum oxide (1/5/16)	Mo5 O16 Te	96-100-1809	0.7962
Porphyrazinealuminiumchloride	C16 Al Cl N16 S4	96-430-9965	0.7911
	C4 Cl2 N4 S4	96-431-9733	0.7893
BSe	C4 Cl2 N4 S4	96-432-0206	0.7893
	C4 Br4 Se	96-210-2931	0.7864
Iron Fluoride	F3 Fe	96-210-0657	0.7853
Barium palladium selenostannate selenide	Ba8 Pd Se18.25 Sn4	96-220-1131	0.7841
	Ag7 Ge I Se5	96-210-3087	0.7840
\alpha-Zn4Sb3	Sb10 Zn13	96-411-3279	0.7838
	C2 F N O S	96-431-7198	0.7838
Laihunite	Fe4.74 O12 Si3	96-900-1036	0.7838
	C4 Cl3 N2 O4 S4	96-411-6448	0.7837
deuterated barium niyroxide	Ba D2 O2	96-210-370	0.7830



	C22 F14	96-411-27150.7835	
	Li2 Mg2 Mo3 O12	96-720-46070.7830	
Enstatite	Al0.03 Fe0.15 Mg1.82 O6 Si1.97	96-901-0890	0.7830
Albite	Al1.02 Ca0.02 Na0.98 O8 Si2.98	96-900-9664	0.7827
Trilithium aluminium trimolybdate(VI)	Al Li3 Mo3 O12	96-201-8503	0.7826
	Bi5.91 La2.1 Pb2 S14	96-431-9504	0.7824
Galenobismutite	Bi2 Pb S4	96-901-09200.7822	
Copper iron molybdate (1.82/1.82/3)	Cu1.815 Fe1.815 Mo3 O12	96-200-2745	0.7821
deuterated barium hydroxide	Ba D2 O2	96-210-37600.7821	
Wood	C8 K4 N4 O8 S8	96-715-14770.7821	
	Bi O9 Sm W2	96-701-62380.7818	
	Cu K2 O10 Si4	96-900-97110.7817	
iron tungsten nitride	Fe3 N W3	96-200-67760.7816	
Tetrazink bis(arsenate(V)) oxide - LT	As2 O9 Zn4	96-200-2751	0.7813
	Cu In Se	96-410-52940.7813	
	Al F6 K3	96-430-33200.7813	
	C12 Br6 O4	96-430-48040.7813	
Barium	Ba	96-900-85300.7812	
Silver lead tris(dibismuth/antimony) hexasulfide	Ag Bi1.998 Pb S6 Sb0.911	96-201-7383	0.7811
Albite	Al Na O8 Si3	96-900-07080.7811	
	Al1.45 Na1.45 O4 Si0.55	96-200-2898	0.7810
	Al1.45 Na1.45 O4 Si0.55	96-200-2899	0.7810
Anorthite	Al2 Ca O8 Si2	96-900-12590.7810	
Lanthanum molybdenum oxide (7/7/30)	La7 Mo7 O30	96-100-0501	0.7809
Monoclinic titanium metaphosphate	O27 P9 Ti3	96-201-0156	0.7809
	Se5 Sn Sr2	96-400-04050.7808	
Barium calcium cobalt iron(III) fluoride (2/1.1/0.9/2/14)	Ba2 Ca1.072 Co0.928 F14 Fe2	96-100-8493	0.7807
Dibarium oxovanadium bis(phosphate(V))	Ba2 O9 P2 V	96-200-2795	0.7806
Dibarium oxovanadium bis(phosphate(V))	Ba2 O9 P2 V	96-200-2810	0.7806
	As 5 Ba2 In5	96-400-12540.7805	
	Ga5.54 La3 O14 Ta0.46	96-210-3502	0.7803
	Ba7 Se11.9 Sn3 Te1.1	96-400-0616	0.7803
	C12 Cl10	96-500-00250.7803	
Anorthoclase	Al K0.333 Na0.667 O8 Si3	96-900-0856	0.7801
Diopside-subsilicic	Ca Fe0.759 Mg0.641 O6 Si1.2	96-900-5341	0.7800
Magnesium iron calcium aluminium silicate * (Augite)	Al0.7 Ca Fe0.2 Mg0.6 O6 Si1.5	96-120-0007	0.7799
Enstatite	Mg O3 Si	96-900-63410.7799	

and 152 others...

[Search-Match](#)

Settings

Reference database used COD-Inorg  
 REV81284 2013.04.15 Automatic zeropoint  
 adaptation Yes

Minimum figure-of-merit (FoM) 0.60  
Parameter/influence 2theta 0.50  
Parameter/influence intensities 0.50  
Parameter multiple/single phase(s) 0.50

## Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	20.19	4.3937	31.06	0.1600	A,B
2	20.31	4.3692	28.94	0.1600	A,C
3	20.46	4.3365	40.11	0.1600	A
4	20.68	4.2906	28.50	0.1600	A
5	20.84	4.2582	27.12	0.1600	A
6	21.07	4.2125	43.86	0.1600	
7	21.20	4.1877	39.61	0.1600	
8	21.47	4.1346	108.72	0.1600	A
9	21.76	4.0807	30.12	0.1600	
10	22.00	4.0372	39.41	0.1600	A,C
11	22.75	3.9057	64.41	0.1600	A
12	22.88	3.8833	23.08	0.1600	A
13	23.23	3.8255	25.35	0.1600	A,C
14	23.46	3.7898	70.05	0.1600	A,C
15	23.74	3.7452	88.93	0.1600	A
16	24.01	3.7030	91.24	0.1600	A
17	24.23	3.6700	33.47	0.1600	A,C
18	24.36	3.6509	27.43	0.1600	A,B,C
19	24.66	3.6070	68.98	0.1600	A
20	24.79	3.5893	69.98	0.1600	
21	25.08	3.5472	234.54	0.1600	A
22	25.31	3.5164	53.13	0.1600	A
23	25.47	3.4948	54.35	0.1600	A,C
24	25.87	3.4406	124.76	0.1600	A,C
25	26.01	3.4225	134.62	0.1600	A
26	26.64	3.3433	400.95	0.1600	A,B,C
27	26.93	3.3079	96.95	0.1600	C
28	27.16	3.2807	135.53	0.1600	A
29	27.50	3.2412	337.79	0.1600	A,B
30	27.82	3.2047	1000.00	0.1600	A,C
31	28.24	3.1571	57.53	0.1600	A,C
32	28.41	3.1388	47.13	0.1600	A
33	28.55	3.1243	31.80	0.1600	A
34	29.62	3.0133	132.93	0.1600	A
35	29.96	2.9805	246.59	0.1600	A,B
36	30.09	2.9673	244.24	0.1600	A,C
37	30.38	2.9402	175.57	0.1600	A,B,C
38	30.66	2.9134	225.56	0.1600	A,C
39	30.87	2.8943	184.74	0.1600	A,B
40	31.31	2.8548	58.22	0.1600	A,C
41	31.60	2.8293	61.13	0.1600	A,B,C

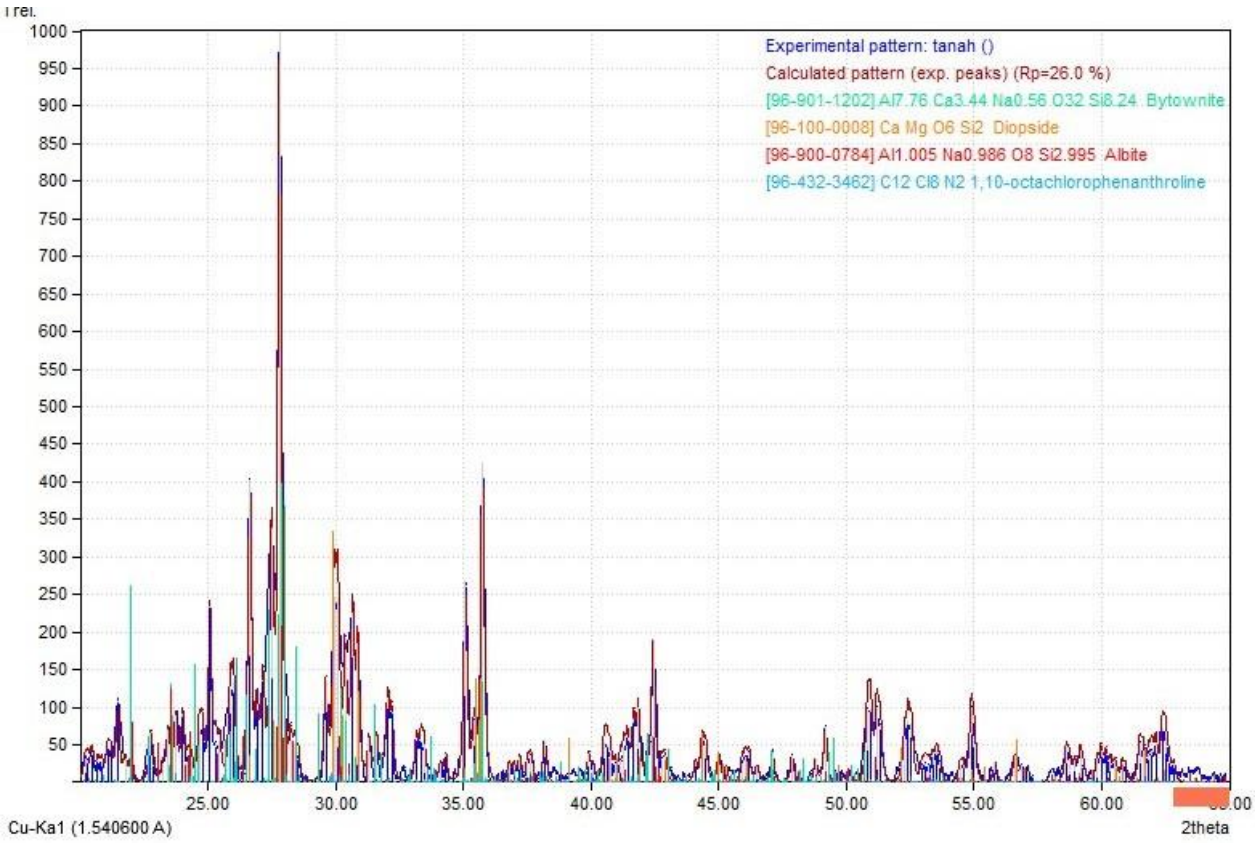
42	31.81	2.8105	21.52	0.1600	A
43	32.04	2.7916	112.52	0.1600	A,C
44	32.20	2.7774	92.05	0.1600	A,C
45	33.17	2.6983	58.19	0.1600	A
46	33.34	2.6852	55.08	0.1600	A,C
47	33.47	2.6753	49.92	0.1600	A,C
48	34.11	2.6264	24.45	0.1600	A,C
49	34.31	2.6113	36.28	0.1600	A
50	35.08	2.5561	267.05	0.1600	A,B,C
51	35.43	2.5313	82.30	0.1600	A,B,C
52	35.76	2.5091	425.68	0.1600	A,B,C
53	36.80	2.4403	24.87	0.1600	A,C
54	37.00	2.4279	22.14	0.1600	A,C
55	37.22	2.4141	33.45	0.1600	A,C
56	37.53	2.3947	27.87	0.1600	A,C
57	37.65	2.3871	35.45	0.1600	A,B,C
58	38.18	2.3550	56.62	0.1600	A,B,C
59	39.91	2.2568	38.17	0.1600	A,C
60	40.09	2.2472	23.31	0.1600	A,C
61	40.51	2.2253	53.69	0.1600	A,B,C
62	40.62	2.2192	49.30	0.1600	A,B
63	40.75	2.2126	41.01	0.1600	A,B
64	40.95	2.2021	25.47	0.1600	A,B
65	41.15	2.1920	28.70	0.1600	A,C
66	41.29	2.1849	45.35	0.1600	A,C
67	41.43	2.1775	57.96	0.1600	A
68	41.67	2.1655	83.22	0.1600	A
69	41.85	2.1566	98.44	0.1600	A,B,C
70	42.19	2.1400	27.83	0.1600	A,C
71	42.44	2.1282	189.12	0.1600	A,B,C
72	42.76	2.1132	29.21	0.1600	A,C
73	42.90	2.1063	35.99	0.1600	A,B,C
74	44.10	2.0520	27.67	0.1600	A,C
75	44.35	2.0408	58.84	0.1600	A,B
76	44.50	2.0344	50.94	0.1600	A,C
77	45.01	2.0123	36.17	0.1600	A,B,C
78	45.29	2.0005	20.96	0.1600	A,B,C
79	45.92	1.9747	25.39	0.1600	A,C
80	46.04	1.9697	33.76	0.1600	A,B,C
81	46.19	1.9639	38.93	0.1600	A,C
82	46.51	1.9508	21.15	0.1600	A,B,C
83	47.12	1.9270	39.66	0.1600	A,C
84	47.87	1.8988	35.37	0.1600	A,B,C
85	48.79	1.8651	30.60	0.1600	A,B,C
86	49.18	1.8511	73.57	0.1600	A,C
87	50.83	1.7948	97.69	0.1600	A,B,C
88	50.95	1.7910	97.30	0.1600	A
89	51.20	1.7829	99.87	0.1600	A,C
90	51.33	1.7786	76.60	0.1600	B,C
91	52.28	1.7484	57.85	0.1600	B,C
92	52.41	1.7443	81.95	0.1600	C
93	52.55	1.7400	77.68	0.1600	C
94	52.97	1.7274	22.33	0.1600	C
95	53.09	1.7237	24.44	0.1600	C
96	53.21	1.7201	21.98	0.1600	B,C
97	53.38	1.7151	32.42	0.1600	C
98	53.54	1.7103	40.78	0.1600	B
99	53.67	1.7063	27.19	0.1600	C
100	54.45	1.6838	22.05	0.1600	B,C
101	54.57	1.6803	22.54	0.1600	C
102	54.89	1.6713	98.27	0.1600	B,C
103	55.00	1.6681	60.05	0.1600	C
104	55.82	1.6456	25.59	0.1600	C
105	56.60	1.6249	36.24	0.1600	B,C
106	56.85	1.6183	23.25	0.1600	B
107	58.60	1.5739	45.56	0.1600	B,C
108	58.73	1.5709	31.82	0.1600	C
109	58.95	1.5655	28.29	0.1600	C
110	59.16	1.5604	40.78	0.1600	B,C
111	59.27	1.5577	21.22	0.1600	B,C
112	59.81	1.5450	30.93	0.1600	B,C
113	59.98	1.5410	42.23	0.1600	B,C
114	60.17	1.5367	37.35	0.1600	C
115	60.35	1.5325	27.66	0.1600	C
116	60.53	1.5284	27.84	0.1600	B,C
117	60.79	1.5224	25.25	0.1600	B,C
118	60.93	1.5194	21.03	0.1600	C
119	61.49	1.5068	52.52	0.1600	B,C

120	61.62	1.5040	41.47	0.1600	B,C
121	61.83	1.4992	37.49	0.1600	C
122	61.97	1.4963	41.86	0.1600	B,C
123	62.12	1.4929	52.60	0.1600	B,C
124	62.37	1.4876	71.05	0.1600	C
125	62.49	1.4851	58.73	0.1600	B,C
126	62.62	1.4822	28.79	0.1600	C
127	62.82	1.4781	24.50	0.1600	C

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Diffraction Pattern Graphics



## Match! Phase Analysis Report

### Sample: 3B#mhs#S1#2020

**Sample Data**  
File name 3B#mhs#S1#2020.txt  
File path D:/Data/App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/3B#mhs#S1#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 19.920° - 64.900°  
Number of points 2251  
Step size 0.020  
Rietveld refinement converged

No Alpha2 subtracted

Y

es  
Background subtr. Yes  
Data smoothed Yes  
2theta correction -0.08°  
Radiation X-rays  
Wavelength 1.540598 Å

### Matched Phases

Index	Amount (%)	Name	Formula sum
A	50.7	Pigeonite	Ca0.106 Fe0.419 Mg0.461 Mn0.014 O3 Si
B	27.3	Albite	Al Na O8 Si3
C	22.0	Diopside	Ca Mg O6 Si2

#### A: Pigeonite (50.7 %)

Formula sum Ca0.106 Fe0.419 Mg0.461 Mn0.014 O3 Si

Entry number 96-900-7054

Figure-of-Merit (FoM)0.813716

Total number of peaks459

Peaks in range 143

Peaks matched 120

Intensity scale factor 0.89

Space group P 1 21/c 1

Crystal system monoclinic

Unit cell a= 9.8010 Å b= 9.0080 Å c= 5.2960 Å β= 109.010 °

I/Icor 1.17

Calc. density 3.475 g/cm<sup>3</sup>

Reference Camara F., Carpenter M. A., Domeneghetti M. C., Tazzoli V., "Non-convergent ordering and displacive phase transition in pigeonite: in situ HT XRD study Sample: hgd, T = 650 C", Physics and Chemistry of Minerals **29**, 331-340 (2002)

#### B: Albite (27.3 %)

Formula sum Al Na O8 Si3

Entry number 96-900-3702  
 Figure-of-Merit (FoM) 0.826422  
 Total number of peaks 253  
 Peaks in range 189  
 Peaks matched 172  
 Intensity scale factor 0.35  
 Space group C -1  
 Crystal system triclinic (anorthic)  
 Unit cell  $a = 7.5713 \text{ \AA}$   $b = 12.5170 \text{ \AA}$   $c = 6.9697 \text{ \AA}$   $\alpha = 93.797^\circ$   $\beta = 117.448^\circ$   $\gamma = 87.508^\circ$   
 I/Icor 0.86  
 Calc. density  $2.978 \text{ g/cm}^3$   
 Reference Benusa M. D., Angel R. J., Ross N. L., "Compression of albite, NaAlSi<sub>3</sub>O<sub>8</sub> Sample: Amelia Court House, Virginia locality P = 8.411 GPa", American Mineralogist **90**, 1115-1120 (2005)

**C: Diopside (22.0 %)**

Formula sum Ca Mg O6 Si2  
 Entry number 96-100-0010  
 Figure-of-Merit (FoM) 0.793845  
 Total number of peaks 221  
 Peaks in range 72  
 Peaks matched 68  
 Intensity scale factor 0.41  
 Space group C 1 2/c 1  
 Crystal system monoclinic  
 Unit cell  $a = 9.6808 \text{ \AA}$   $b = 8.8488 \text{ \AA}$   $c = 5.2180 \text{ \AA}$   $\beta = 105.606^\circ$   
 I/Icor 1.25  
 Calc. density  $3.341 \text{ g/cm}^3$   
 Reference Thompson R. M., Downs R. T., "The crystal structure of diopside at pressure to 10 GPa Locality: DeKalb, New York Sample: P = 2.32 GPa", American Mineralogist **93**, 177-186 (2008)

**Candidates**

Name	Formula	Entry No.	FoM
	D0.83 Nb	96-411-1971	0.8190
	Ge	96-710-1739	0.8123
	Ge	96-710-1740	0.7942
\alpha-Zn <sub>4</sub> Sb <sub>3</sub>	Sb <sub>10</sub> Zn <sub>13</sub>	96-411-3279	0.7920
Rhodium(III) copper oxide	Cu O <sub>2</sub> Rh	96-100-8163	0.7888
	C <sub>19</sub> Er <sub>10</sub> Ru <sub>10</sub>	96-200-3120	0.7862
trizirconium nickel heptaantimonide	Ni Sb <sub>7</sub> Zr <sub>3</sub>	96-221-9187	0.7787
beta-Tricalcium nitrido dialuminate	Al <sub>2</sub> Ca <sub>3</sub> N <sub>4</sub>	96-432-1679	0.7773
Jerrygibbsite	H <sub>2</sub> Mn <sub>9</sub> O <sub>18</sub> Si <sub>4</sub>	96-901-1748	0.7746
	Ca <sub>3</sub> Ce <sub>2</sub> Ge <sub>4</sub>	96-411-2075	0.7731
Nonastrontium tetrazinc dicopper(I) oxide	Cu <sub>2</sub> O <sub>14</sub> Sr <sub>9</sub> Zn <sub>4</sub>	96-200-2521	0.7724
	La <sub>4</sub> P <sub>9</sub> Rh <sub>8</sub>	96-432-4797	0.7713
Laihunite	Fe <sub>4.74</sub> O <sub>12</sub> Si <sub>3</sub>	96-900-1036	0.7699
Neon	Ne	96-901-1726	0.7694
	Ag <sub>14.814</sub> Cu <sub>1.186</sub> Si <sub>11</sub> Sb <sub>2</sub>	96-210-0480	0.7693

Polybasite	Ag <sub>29.629</sub> Cu <sub>2.371</sub> S <sub>22</sub> Sb <sub>4</sub>	96-901-1313	0.7693
Bismuth strontium copper oxide (4/7.9/5/19.1)	Bi <sub>4</sub> Cu <sub>5</sub> O <sub>19.06</sub> Sr <sub>7.86</sub>	96-100-6050	0.7684
	Ca <sub>3.2</sub> Ce <sub>1.8</sub> Ge <sub>4</sub>	96-411-2074	0.7661
Silver cadmium (0.49/0.51) - HT	Ag <sub>0.49</sub> Cd <sub>0.51</sub>	96-150-9122	0.7660
Ramdohrite	Ag <sub>1.5</sub> Pb <sub>3</sub> S <sub>12</sub> Sb <sub>5.5</sub>	96-901-1731	0.7660
Janhaugite	Ca <sub>0.69</sub> F <sub>2</sub> Mn <sub>3</sub> Na <sub>2.31</sub> O <sub>16</sub> Si <sub>4</sub> Ti <sub>1.4</sub> Zr <sub>0.696</sub>	96-900-9321	0.7659
Strontium divanadium(III) oxide bis(phosphate(V))	O <sub>9</sub> P <sub>2</sub> Sr V <sub>2</sub>	96-100-1749	0.7647
Platinum	Pt	96-101-1115	0.7644
Silver Silicate Chloride	Ag <sub>20</sub> Cl <sub>4</sub> O <sub>16</sub> Si <sub>4</sub>	96-810-3015	0.7644
	Ga <sub>2</sub> O <sub>9</sub> Zn <sub>6</sub>	96-210-4211	0.7637
Wollastonite-2M	Ca O <sub>3</sub> Si	96-901-1914	0.7630
	Ga <sub>6</sub> O <sub>19</sub> Sr <sub>10</sub>	96-210-4469	0.7628
Fizelyite	Ag <sub>1.486</sub> Pb <sub>3.436</sub> S <sub>12</sub> Sb <sub>5.215</sub>	96-901-3807	0.7625
Palladium	Pd	96-101-1106	0.7623
Sillimanite	Al <sub>2</sub> O <sub>5</sub> Si	96-900-6528	0.7619
Ce <sub>20</sub> Au <sub>1.72</sub> Ge <sub>14.28</sub>	Au <sub>0.43</sub> Ce <sub>5</sub> Ge <sub>3.58</sub>	96-220-5826	0.7618
	Ca <sub>1.74</sub> Ce <sub>3.26</sub> Ge <sub>4</sub>	96-411-2073	0.7618
	Mn Sb <sub>2</sub> Sr <sub>2</sub>	96-430-9154	0.7616
Sillimanite	Al <sub>2</sub> O <sub>5</sub> Si	96-900-3987	0.7611
Leucite	Al O <sub>6</sub> Rb Si <sub>2</sub>	96-900-1797	0.7605
Zirconolite	Ca <sub>2</sub> O <sub>14</sub> Ti <sub>4</sub> Zr <sub>2</sub>	96-900-9221	0.7603
TELLURIUM(VI) HYDROXIDE TETRACAESIUM HYDROGENPHOSPHATE BIS(DIHYDROGENPHOSPHATE)Cs <sub>4</sub> H <sub>11</sub> O <sub>18</sub> P <sub>3</sub> Te		96-100-7141	0.7601
	Cu <sub>2</sub> S <sub>2</sub> Sm <sub>2</sub> Te <sub>2</sub>	96-432-2571	0.7600
Calcium Silicon Nitride	Bi <sub>6</sub> Cl Fe O <sub>14</sub> Ti <sub>2</sub>	96-400-1695	0.7598
Cannizzarite	Ca <sub>8</sub> N <sub>16</sub> Si <sub>8</sub>	96-431-1198	0.7592
Palladium	Bi <sub>54</sub> Pb <sub>46</sub> S <sub>127</sub>	96-901-1203	0.7592
BARIUM TANTALUM TITANIUM OXIDE (3/3.2/5/21)	Pd	96-101-1107	0.7591
Periclase	Ba <sub>3</sub> O <sub>21</sub> Ta <sub>3.2</sub> Ti <sub>5</sub>	96-100-1305	0.7585
	Mg O	96-900-6772	0.7582
	Ga <sub>6</sub> O <sub>25</sub> Sc <sub>4</sub> Sr <sub>10</sub>	96-432-8033	0.7580
	Co <sub>4</sub> Ge <sub>12</sub> In Yb <sub>7</sub>	96-400-1442	0.7572
strontium tellurite	O <sub>3</sub> Sr Te	96-221-4075	0.7571
	Sb <sub>3</sub> Tm <sub>5</sub>	96-430-2123	0.7571
Palladium	Pd	96-901-2963	0.7571
	In <sub>9</sub> Li <sub>2</sub> Y <sub>5</sub>	96-430-9585	0.7570
	La <sub>6</sub> O <sub>18</sub> W <sub>3</sub>	96-450-1293	0.7570
	Se <sub>9</sub> Sn <sub>2</sub> Sr <sub>4</sub>	96-431-1784	0.7565

and 154 others...

## Search-Match

### Settings

Reference database used	COD-Inorg REV81284 2013.04.15
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

## Peak List

No.	2theta [°]	d [Å]	I/I <sub>0</sub>	FWHM	Matched
1	23.41	3.7973	103.32	0.4798	
2	23.52	3.7802	96.57	0.4798	A,B
3	24.07	3.6940	100.04	0.4798	C
4	24.78	3.5901	281.93	0.4798	A,B
5	24.92	3.5699	286.88	0.4798	B
6	25.63	3.4727	375.44	0.4798	B
7	26.62	3.3462	372.33	0.4798	A,B,C
8	27.46	3.2454	1000.00	0.4798	A,B,C
9	29.66	3.0095	909.61	0.4798	A,B
10	30.16	2.9610	769.52	0.4798	A,B,C
11	30.77	2.9035	373.23	0.4798	A,B,C
12	30.92	2.8900	411.15	0.4798	
13	31.08	2.8750	385.98	0.4798	C
14	31.22	2.8622	404.90	0.4798	A
15	31.45	2.8421	367.27	0.4798	B
16	31.85	2.8074	523.30	0.4798	A,B,C
17	33.41	2.6798	236.14	0.4798	B
18	33.62	2.6635	236.03	0.4798	
19	33.76	2.6530	235.42	0.4798	A
20	34.02	2.6330	230.40	0.4798	
21	34.80	2.5756	637.70	0.4798	A,B
22	35.14	2.5520	766.96	0.4798	A
23	35.36	2.5362	784.33	0.4798	A,B,C
24	37.01	2.4273	318.71	0.4798	A,B
25	37.25	2.4121	278.86	0.4798	
26	37.43	2.4004	311.25	0.4798	A,B

27	38.18	2.3554	95.71	0.4798	A,B,C
28	38.38	2.3436	111.64	0.4798	A,B
29	38.55	2.3335	132.81	0.4798	B,C
30	38.79	2.3196	166.89	0.4798	A,B
31	38.98	2.3089	153.43	0.4798	B
32	39.29	2.2910	94.92	0.4798	B,C
33	39.64	2.2716	96.89	0.4798	A,B
34	39.80	2.2632	110.21	0.4798	B
35	39.96	2.2545	129.02	0.4798	A,B
36	40.15	2.2439	91.76	0.4798	A
37	40.75	2.2125	103.81	0.4798	B,C
38	41.12	2.1934	157.79	0.4798	A,B,C
39	41.65	2.1665	792.76	0.4798	A
40	42.59	2.1210	98.78	0.4798	A,B,C
41	42.77	2.1126	135.15	0.4798	B,C

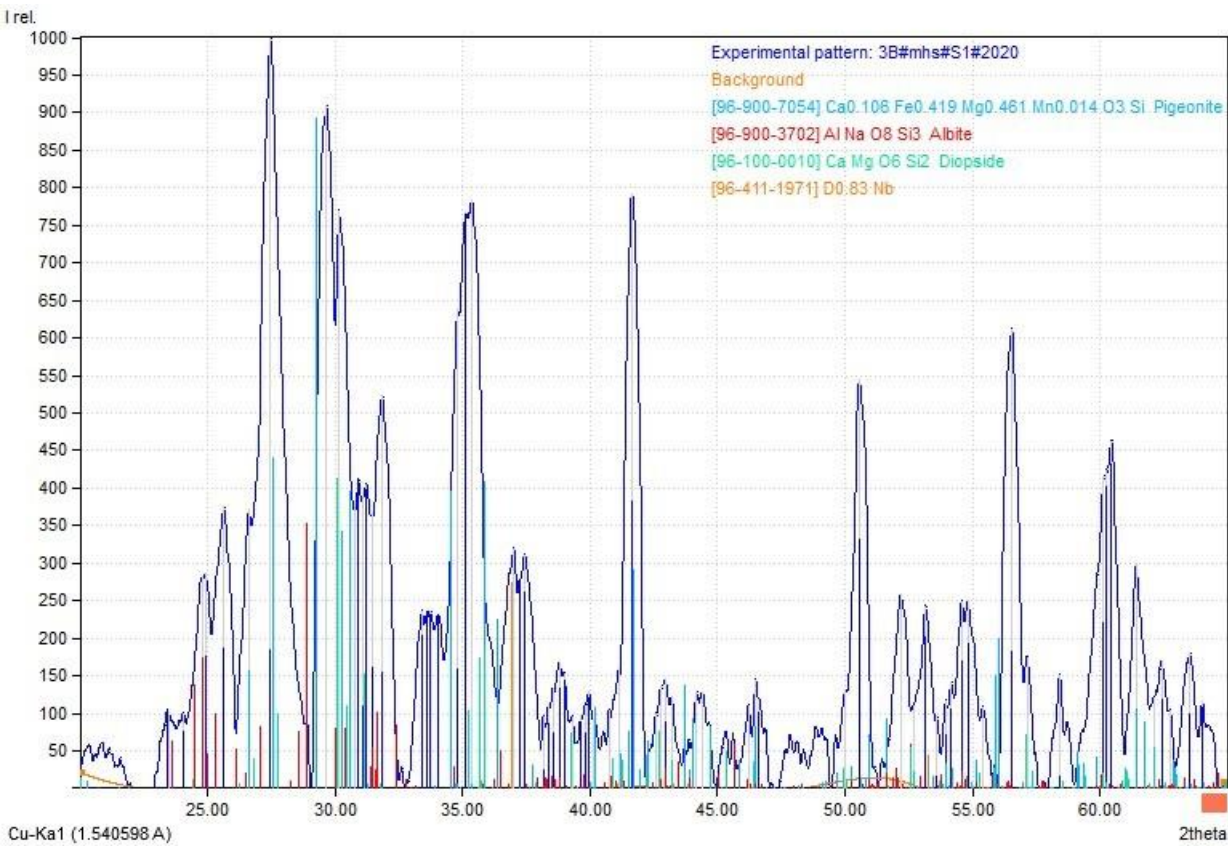


42	42.95	2.1041	146.77	0.4798	A,B
43	43.20	2.0927	122.45	0.4798	A,B,C
44	44.18	2.0484	127.96	0.4798	A,B,C
45	44.41	2.0381	128.95	0.4798	A,B,C
46	46.21	1.9630	110.56	0.4798	A,B,C
47	46.49	1.9517	144.65	0.4798	A,B,C
48	46.62	1.9466	118.44	0.4798	A,B,C
49	50.02	1.8222	130.27	0.4798	A,B,C
50	50.56	1.8037	543.82	0.4798	A,B,C
51	52.17	1.7517	258.52	0.4798	A,B,C
52	52.67	1.7365	110.17	0.4798	A,B,C
53	53.17	1.7213	242.31	0.4798	B
54	53.60	1.7084	96.22	0.4798	A,B,C
55	53.94	1.6984	116.80	0.4798	A,C
56	54.17	1.6919	141.09	0.4798	A,B
57	54.58	1.6801	248.42	0.4798	B
58	54.82	1.6734	249.65	0.4798	A,B,C
59	55.40	1.6571	107.59	0.4798	A,B,C
60	56.53	1.6267	610.69	0.4798	A,B
61	57.13	1.6109	174.10	0.4798	A,B,C
62	58.42	1.5783	150.15	0.4798	A,B,C
63	60.14	1.5374	414.99	0.4798	A,B,C
64	60.27	1.5344	422.85	0.4798	A,B
65	60.45	1.5301	462.30	0.4798	A,B,C
66	61.42	1.5083	299.18	0.4798	A,B,C
67	62.11	1.4933	120.62	0.4798	A,B,C
68	62.42	1.4866	169.59	0.4798	A,B,C
69	62.75	1.4795	103.78	0.4798	A,B,C
70	63.53	1.4632	179.13	0.4798	A,B,C
71	64.00	1.4535	115.27	0.4798	A,C

## Rietveld Refinement using FullProf

Calculation was not run or did not converge.

## Diffraction Pattern Graphics



# Match! Phase Analysis Report

## Sample: batuan ()

**Sample Data**  
File name 4C#mhs#S1#2020.ORG  
File path D:/Data/App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/4C#mhs#S1#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 20.010° - 65.010°  
Number of points 2251  
Step size 0.020  
Rietveld refinement converged

No Alpha2 subtracted

No  
Background subtr. No  
Data smoothed No  
2theta correction 0.01°  
Radiation X-rays  
Wavelength 1.540600 Å

## Matched Phases

Index	Amount (%)	Name	Formula sum
A	90.1	Anorthite	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	9.9	Pigeonite	Al <sub>0.02</sub> Ca <sub>0.121</sub> Fe <sub>1.008</sub> Mg <sub>0.871</sub> O <sub>6</sub> Si <sub>1.98</sub>

### A: Anorthite (90.1 %)

Formula sum Al<sub>2</sub> Ca O<sub>8</sub> Si<sub>2</sub>  
Entry number 96-900-1174  
Figure-of-Merit (FoM) 0.789641  
Total number of peaks 247  
Peaks in range 231  
Peaks matched 53  
Intensity scale factor 0.45  
Space group I -1  
Crystal system triclinic (anorthic)  
Unit cell a= 8.0420 Å b= 12.7480 Å c= 13.9640 Å α= 92.200° β= 115.270 ° γ= 92.650 °  
I/I<sub>cor</sub> 0.61  
Calc. density 2.862 g/cm<sup>3</sup>  
Reference Angel R. J., "High-pressure structure of anorthite Sample: P = 31 kbar", American Mineralogist **73**, 1114-1119 (1988)

### B: Pigeonite (9.9 %)

Formula sum Al<sub>0.02</sub> Ca<sub>0.121</sub> Fe<sub>1.008</sub> Mg<sub>0.871</sub> O<sub>6</sub> Si<sub>1.98</sub>  
Entry number 96-901-3712  
Figure-of-Merit (FoM) 0.618116

Total number of peaks 431  
 Peaks in range 140  
 Peaks matched 31  
 Intensity scale factor 0.05  
 Space group P 1 21/c 1  
 Crystal system monoclinic  
 Unit cell a= 9.6220 Å b= 8.8610 Å c= 5.1810 Å β= 107.920 °  
 I/Icor 1.15  
 Calc. density 3.705 g/cm<sup>3</sup>  
 Reference Alvaro M., Nestola F., Ballaran T. B., Camara F., Domeneghetti M. C., Tazzoli V.,  
 "High-pressure phase transition of a natural pigeonite Locality: Parana, Brazil  
 Note: P = 3.172 GPa", American Mineralogist **95**, 300-311 (2010)

## Candidates

Name	Formula	Entry No.	FoM
	B3 H3 N12	96-432-2188	0.7715
Silver indium antimony telluride (0.034/0.037/0.764/0.165)	Ag0.034 In0.037 Sb0.764 Te0.165	96-150-9071	0.7396
Tungsten	W	96-900-6511	0.7342
Tungsten	W	96-900-6513	0.7323
Tungsten	W	96-900-6512	0.7306
	Cl3 Cu Nd4 O15 Te5	96-430-9287	0.7235
	Cu2 O7 P2	96-900-7765	0.7185
Iron	Fe	96-901-3479	0.7098
Iron	Fe	96-901-3480	0.7098
Iron	Fe	96-901-3481	0.7056
Vanadium(V) oxide arsenate(V)	As O5 V	96-222-9494	0.7016
	Bi2 Hf2 O7	96-400-1329	0.7007
Iron	Fe	96-901-3482	0.7006
Thallium niobium oxide (10/29.2/78)	Nb29.2 O78 Tl10	96-100-1326	0.6899
Lanthanum molybdate oxide	La4 Mo7 O27	96-222-2914	0.6879
Iron	Fe	96-901-3483	0.6832
Strontium carbonate (Strontianite)	C O3 Sr	96-500-0094	0.6789
Muckeite	Bi0.9 Cu Ni S3 Sb0.1	96-900-7732	0.6775
Discandium disilicate (Thortveitite)	O7 Sc2 Si2	96-101-1148	0.6774
Strontianite	C O3 Sr	96-900-0228	0.6764
Lautarite	Ca I2 O6	96-901-1187	0.6762
Lithium Aluminum Boron Oxide (2/1/5/10)	AlB5 Li2 O10	96-110-0062	0.6753
Esperanzaite	Al2 As2 Ca2 F4 H5 Na0.68 O11	96-900-4518	0.6750
Cerium sulfide iodide - α	Ce I S	96-100-8317	0.6699
Iron	Fe	96-901-3484	0.6698
	B7 H5 O14 Rb2	96-430-0576	0.6692
Periclase	Mg O	96-901-3251	0.6683
cesium-lithium phyllosilicate	Cs1.33 Li0.67 O5 Si2	96-200-3993	0.6639
Dicaesium tecto-hydroxotrichromatoarsenate	As Cr3 Cs 2 H O13	96-100-1561	0.6638
Periclase	Mg O	96-901-3198	0.6637
	Ba2 Dy Ga Se5	96-432-9517	0.6617
	Fe	96-720-4905	0.6607
Iron	Fe	96-901-3477	0.6602

Uklonskovite	F H4 Mg Na O6 S	96-901-20900.6590
Silver aluminum (0.75/0.25) - HT	Ag0.75 Al0.25	96-150-90330.6565
Rubidium tetrafluoroaluminate	Al F4 Rb	96-100-04540.6554
Sodium strontium diarsenidodistannate (0.4/0.6/1)	As2 Na0.4 Sn2 Sr0.6	96-100-8734 0.6554
Magnesiowuestite	Fe0.4 Mg0.6 O	96-900-60990.6537
Rubidium tetrafluoroaluminate	Al F4 Rb	96-100-04550.6525
Zinc catena-polyphosphate	O6 P2 Zn	96-201-37390.6495
Magnesiowuestite	Fe0.4 Mg0.6 O	96-900-60680.6440
	In K O6 Se2	96-432-99670.6421
	Ba2 Ga Se5 Y	96-432-95130.6408
Magnesiowuestite	Fe0.4 Mg0.6 O	96-900-60810.6405
Stalderite	As2 Cu Fe0.46 Hg0.38 S6 Tl Zn1.16	96-901-2870 0.6397
	K Li O4 S	96-210-20930.6380
	B3 H Li Na O8 Si	96-210-28390.6365
	Cr Sb	96-900-88900.6355
Magnesiowuestite	Fe0.4 Mg0.6 O	96-900-60540.6337
Iron	Fe	96-901-34780.6305
Leiteite	As2 O4 Zn	96-900-10720.6290
Magnesiowuestite	Fe0.4 Mg0.6 O	96-900-61000.6287
<i>and 17 others...</i>		

#### Search-Match

#### Settings

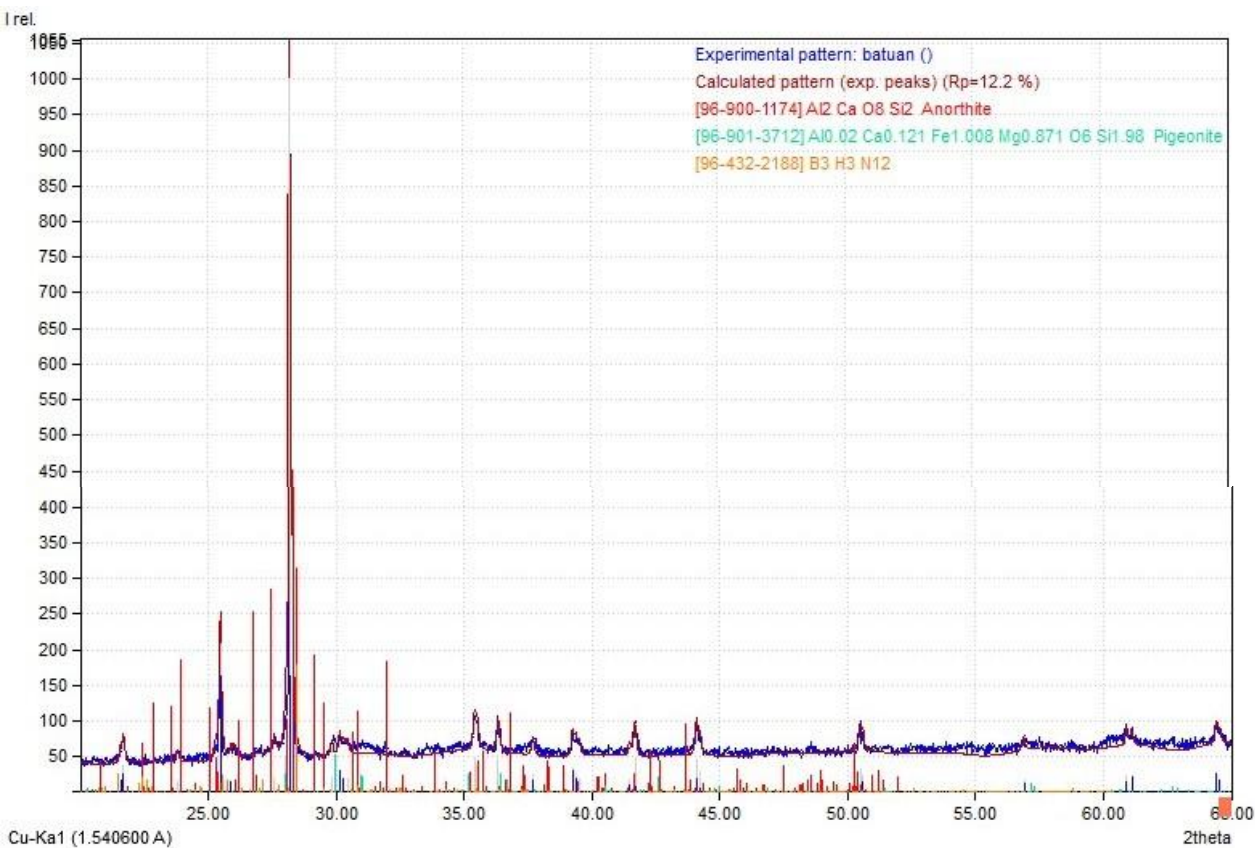
Reference database used COD-Inorg  
REV81284 2013.04.15 Automatic zeropoint  
adaptation Yes  
Minimum figure-of-merit (FoM) 0.60  
Parameter/influence 2theta 0.50  
Parameter/influence intensities 0.50  
Parameter multiple/single phase(s) 0.50

## Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	21.58	4.1154	17.53	0.1200	
2	21.69	4.0934	36.87	0.1200	A,B
3	23.80	3.7353	16.25	0.1200	A
4	25.29	3.5193	18.02	0.1200	A,B
5	25.47	3.4938	207.37	0.1200	A
6	25.89	3.4382	16.75	0.1200	A
7	26.04	3.4195	16.14	0.1200	A
8	27.59	3.2304	19.92	0.1200	A
9	28.04	3.1799	48.96	0.1200	A,B
10	28.21	3.1605	1000.00	0.1200	A
11	29.83	2.9926	20.58	0.1200	A,B
12	30.15	2.9621	29.72	0.1200	
13	30.28	2.9489	19.49	0.1200	
14	30.44	2.9346	19.88	0.1200	A,B
15	35.42	2.5324	48.70	0.1200	A,B
16	35.52	2.5252	36.14	0.1200	A,B
17	36.33	2.4709	46.51	0.1200	A,B
18	37.70	2.3844	23.75	0.1200	B
19	39.25	2.2933	33.85	0.1200	A,B

20	39.37	2.2868	22.95	0.1200	B
21	39.49	2.2801	18.81	0.1200	A
22	41.48	2.1753	17.69	0.1200	A
23	41.68	2.1650	48.64	0.1200	A,B
24	44.09	2.0521	47.03	0.1200	A
25	44.23	2.0460	28.09	0.1200	A,B
26	50.48	1.8063	33.56	0.1200	A,B
27	50.59	1.8028	24.41	0.1200	A
28	56.90	1.6169	16.25	0.1200	B
29	60.91	1.5197	22.51	0.1200	B
30	61.11	1.5153	22.95	0.1200	B
31	64.42	1.4453	28.80	0.1200	B
32	64.53	1.4429	17.21	0.1200	

### Rietveld Refinement using FullProf



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# Match! Phase Analysis Report

## Sample: batuan ()

**Sample Data**  
File name 5b#mhs#S1#2020.ORG  
File path D:/Data/App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/5b#mhs#S1#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 20.030° - 65.030°  
Number of points 2251  
Step size 0.020  
Rietveld refinement  
converged No Alpha2 subtracted No  
Background subtr. Yes  
Data smoothed Yes  
2theta correction 0.03°  
Radiation X-rays  
Wavelength 1.540600 Å

## Matched Phases

Index	Amount (%)	Name	Formula sum
A	44.3	Anorthite	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	25.7	Albite	Al Ge <sub>2</sub> Na O <sub>8</sub> Si
C	25.5	Pigeonite	Ca <sub>0.15</sub> Mg <sub>1.85</sub> O <sub>6</sub> Si <sub>2</sub>
D	4.4	Magnetite	Fe <sub>3</sub> O <sub>4</sub>

### A: Anorthite (44.3 %)

Formula sum Al<sub>2</sub> Ca O<sub>8</sub> Si<sub>2</sub>  
Entry number 96-900-0363  
Figure-of-Merit (FoM) 0.847445  
Total number of peaks 500  
Peaks in range 465  
Peaks matched 315  
Intensity scale factor 0.39  
Space group P -1  
Crystal system triclinic (anorthic)  
Unit cell a= 8.2230 Å b= 12.9150 Å c= 14.2040 Å α= 92.750° β= 115.800° γ= 91.020°  
I/I<sub>cor</sub> 0.60  
Calc. density 2.725 g/cm<sup>3</sup>  
Reference Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 C T = 830 C", American Mineralogist **58**, 665-675 (1973)

### B: Albite (25.7 %)

Formula sum Al Ge<sub>2</sub> Na O<sub>8</sub> Si  
Entry number 96-900-5079  
Figure-of-Merit (FoM) 0.801389  
Total number of peaks 250  
Peaks in range 231  
Peaks matched 177  
Intensity scale factor 0.43

Space group C -1  
 Crystal system triclinic (anorthic)  
 Unit cell  $a= 8.3258 \text{ \AA}$   $b= 13.1590 \text{ \AA}$   $c= 7.2734 \text{ \AA}$   $\alpha= 94.172^\circ$   $\beta= 116.306^\circ$   $\gamma= 90.693^\circ$   
 I/Icor 1.15  
 Calc. density  $3.278 \text{ g/cm}^3$   
 Reference Kroll H., Flogel J., Breit U., Lons J., Pentinghaus H., "Order and anti-order in Ge-substituted alkali feldspars Sample: Na[AlSiGe<sub>2</sub>O<sub>8</sub>] synthesized at 600 deg C", European Journal of Mineralogy **3**, 739-749 (1991)

**C: Pigeonite (25.5 %)**

Formula sum Ca<sub>0.15</sub> Mg<sub>1.85</sub> O<sub>6</sub> Si<sub>2</sub>  
 Entry number 96-900-5630  
 Figure-of-Merit (FoM) 0.793571  
 Total number of peaks 437  
 Peaks in range 137  
 Peaks matched 98  
 Intensity scale factor 0.35  
 Space group P 1 21/c 1  
 Crystal system monoclinic  
 Unit cell  $a= 9.6510 \text{ \AA}$   $b= 8.8460 \text{ \AA}$   $c= 5.2520 \text{ \AA}$   $\beta= 108.380^\circ$   
 I/Icor 0.95  
 Calc. density  $3.169 \text{ g/cm}^3$   
 Reference Merli M., Camara F., "Topological analysis of the electron density of the clinopyroxene structure by the maximum entropy method: an exploratory study Sample: Dien2 Note: c-cell parameter changed by personal communication with author, Dec 2003", European Journal of Mineralogy **15**, 903-911 (2003)

**D: Magnetite (4.4 %)**

Formula sum Fe<sub>3</sub> O<sub>4</sub>  
 Entry number 96-900-6195  
 Figure-of-Merit (FoM) 0.766931  
 Total number of peaks 35  
 Peaks in range 8  
 Peaks matched 7  
 Intensity scale factor 0.40  
 Space group F d -3 m  
 Crystal system cubic  
 Unit cell  $a= 8.3970 \text{ \AA}$   
 I/Icor 6.22  
 Calc. density  $5.195 \text{ g/cm}^3$   
 Reference O'Neill H St C, Dollase W. A., "Crystal structures and cation distributions in simple spinels from powder XRD structural refinements: MgCr<sub>2</sub>O<sub>4</sub>, ZnCr<sub>2</sub>O<sub>4</sub>, Fe<sub>3</sub>O<sub>4</sub> and the temperature dependence of the cation distribution in ZnAl<sub>2</sub>O<sub>4</sub> Sample: 2B model, Fe<sub>3</sub>O<sub>4</sub>", Physics and Chemistry of Minerals **20**, 541-555 (1994)

# Candidates

Name	Formula	Entry No.	FoM
sodium chloride	Cl Na	96-210-40260.8325	
Ag <sub>2</sub> As <sub>7</sub> Cu <sub>1.5</sub> Pb <sub>19</sub> S <sub>56</sub> Sb <sub>16.5</sub> Porphyrazinealuminiumchloride	Ag <sub>1.86</sub> As <sub>7.06</sub> Bi <sub>0.1</sub> Cu <sub>1.73</sub> Hg <sub>0.24</sub> Pb <sub>19.13</sub> S <sub>56</sub> Sb <sub>16.47</sub> Ti <sub>0.24</sub>	96-210-5250	0.8292
	C <sub>16</sub> Al Cl N <sub>16</sub> S <sub>4</sub>	96-430-9965	0.8276
	C <sub>6</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	96-200-1647	0.8258
strontium tellurite	O <sub>3</sub> Sr Te	96-221-2782	0.8242
Wairauite	Co Fe	96-900-4230	0.8224
strontium tellurite	O <sub>3</sub> Sr Te	96-221-4075	0.8158
strontium tellurate(VI)	O <sub>3</sub> Sr Te	96-221-8901	0.8135
Barium fluoroniobate *	Ba <sub>4</sub> F <sub>12</sub> Nb <sub>2</sub> O <sub>3</sub>	96-100-0325	0.8116
Vurroite	As <sub>4.71</sub> Bi <sub>6.97</sub> Cl <sub>3</sub> Pb <sub>9.6</sub> S <sub>27</sub> Sn <sub>0.72</sub> Te Tl <sub>2</sub>	96-901-0439	0.8057
	Te Tl <sub>2</sub>	96-201-2690	0.8051
Sahlinite	As <sub>2</sub> Cl <sub>4</sub> O <sub>17</sub> Pb <sub>14</sub>	96-901-1820	0.8040
Lead molybdenum oxide: Pb~5~MoO~8~	Mo O <sub>8</sub> Pb <sub>5</sub>	96-201-7542	0.8022
Silver bismuth sulfide (3.5/7.5/13)	Ag <sub>3.5</sub> Bi <sub>7.5</sub> S <sub>13</sub>	96-201-4927	0.8016
Kombatite	Cl <sub>4</sub> O <sub>17</sub> Pb <sub>14</sub> V <sub>2</sub>	96-900-1610	0.7993
Paderaite	Bi <sub>11.34</sub> Cu <sub>7.32</sub> Pb <sub>1.34</sub> S <sub>22</sub>	96-900-4986	0.7988
dicopper(I) triselenostannate(IV)	Cu <sub>2</sub> Se <sub>3</sub> Sn	96-201-7656	0.7977
Kukharenkoite-(La)	C <sub>3</sub> Ba <sub>2</sub> F La O <sub>9</sub>	96-901-2775	0.7959
\alpha-Zn <sub>4</sub> Sb <sub>3</sub>	Sb <sub>10</sub> Zn <sub>13</sub>	96-411-3279	0.7941
	Ag <sub>1.09</sub> Ge <sub>4</sub> Na <sub>6.91</sub> Se <sub>10</sub>	96-430-6893	0.7941
Paderaite	Ag <sub>0.2</sub> Bi <sub>11.34</sub> Cu <sub>7.09</sub> Pb <sub>1.37</sub> S <sub>22</sub>	96-900-4985	0.7936
Neon	Ne	96-901-1713	0.7902
Dibarium tricadmium bis(vanadate) divanadate	Ba <sub>2</sub> Cd <sub>3</sub> O <sub>15</sub> V <sub>4</sub>	96-200-2827	0.7900
Tazieffite	As <sub>6.41</sub> Bi <sub>4.59</sub> Cd <sub>0.5</sub> Cl <sub>4</sub> H <sub>0.48</sub> N <sub>0.12</sub> Pb <sub>10.13</sub> S <sub>26</sub> Sn <sub>0.25</sub>	96-901-3678	0.7898
Ramdohrite	Ag <sub>1.5</sub> Pb <sub>3</sub> S <sub>12</sub> Sb <sub>5.5</sub>	96-901-1731	0.7897
Tribarium dilanthanum pentakis(carbonate) difluoride (Cebaite (La))	Ba <sub>3</sub> F <sub>2</sub> La <sub>2</sub> O <sub>15</sub>	96-100-0472	0.7879
	Ag <sub>14.814</sub> Cu <sub>1.186</sub> S <sub>11</sub> Sb <sub>2</sub>	96-210-0486	0.7876
Polybasite	Ag <sub>29.629</sub> Cu <sub>2.371</sub> S <sub>22</sub> Sb <sub>4</sub> K <sub>2</sub> Mg O <sub>12</sub> Si <sub>5</sub>	96-901-1313	0.7876
	K <sub>2</sub> Mg O <sub>12</sub> Si <sub>5</sub>	96-210-1101	0.7872
Calcium catena-polyphosphate	Ca O <sub>6</sub> P <sub>2</sub>	96-400-1395	0.7857
Tricaesium cyclo-triphosphate telluric acid hydrate	Cs <sub>3</sub> H <sub>8</sub> O <sub>16</sub> P <sub>3</sub> Te	96-100-8369	0.7856
calcium(II) strontium(II) tellurium(IV) oxide (0.55/0.45/1/3)	Ca <sub>0.55</sub> O <sub>3</sub> Sr <sub>0.45</sub> Te	96-210-4345	0.7848
Ca <sub>0.77</sub> Sr <sub>0.23</sub> TeO <sub>3</sub>	Ca <sub>0.77</sub> O <sub>3</sub> Sr <sub>0.23</sub> Te	96-210-4346	0.7839
strontium tellurite	O <sub>3</sub> Sr Te	96-221-2469	0.7833
	Al Cs <sub>2</sub> O <sub>10</sub> P <sub>3</sub>	96-700-9288	0.7833
Cebaite-(Ce)	C <sub>5</sub> Ba <sub>3</sub> Ce <sub>2</sub> F <sub>2</sub> O <sub>15</sub>	96-900-9389	0.7831
Hatrrurite	Ca <sub>27</sub> O <sub>45</sub> Si <sub>9</sub>	96-900-8367	0.7830
Schlegelite	As <sub>3</sub> Bi <sub>7</sub> Mo <sub>1.78</sub> O <sub>24</sub> P <sub>0.16</sub> V <sub>0.06</sub>	96-901-0774	0.7827
Cesium disulfate	Cs <sub>2</sub> O <sub>7</sub> S <sub>2</sub>	96-210-4417	0.7821
Arrojadite-(KFe)	Al Ca F <sub>2</sub> Fe <sub>14</sub> K Na <sub>4</sub> O <sub>48</sub> P <sub>12</sub> Cs <sub>2</sub> Ga O <sub>10</sub> P <sub>3</sub>	96-900-0830	0.7813
	Cs <sub>2</sub> Ga O <sub>10</sub> P <sub>3</sub>	96-700-9289	0.7812
Andorite VI	Ag Pb S <sub>6</sub> Sb <sub>3</sub>	96-900-8386	0.7810
Parasterryite	Ag <sub>4</sub> As <sub>10.23</sub> Pb <sub>20.21</sub> S <sub>58</sub> Sb <sub>13.56</sub> Ba <sub>8</sub> Ga <sub>16</sub> Sb <sub>16</sub>	96-210-5251	0.7807
	Ba <sub>8</sub> Ga <sub>16</sub> Sb <sub>16</sub>	96-431-9983	0.7802
Bismuth molybdenum oxide (26/10/69)	Bi <sub>26</sub> Mo <sub>10</sub> O <sub>69</sub>	96-100-4132	0.7801
Barium indium nitride	Ba <sub>19</sub> In <sub>9</sub> N <sub>9</sub> Hf Se <sub>4</sub> Ti <sub>4</sub>	96-220-4402	0.7801
	Hf Se <sub>4</sub> Ti <sub>4</sub>	96-432-4135	0.7798
	Ga <sub>6</sub> O <sub>19</sub> Sr <sub>10</sub>	96-210-4469	0.7797
Eu~12~Ca~2~MnSb~11~	Ca <sub>2</sub> Eu <sub>12</sub> Mn Sb <sub>11</sub>	96-400-0117	0.7794
Proudite	Bi <sub>18.8</sub> Cu <sub>1.5</sub> Pb <sub>14.5</sub> S <sub>30</sub> Se <sub>14</sub> O <sub>21</sub> Se <sub>6</sub> Sr <sub>4</sub> V <sub>2</sub>	96-900-0516	0.7792
	O <sub>21</sub> Se <sub>6</sub> Sr <sub>4</sub> V <sub>2</sub>	96-432-7891	0.7791
calcium(II) strontium(II) tellurium(IV) oxide (0.77/0.23/1/3) - idealised	Ca O <sub>3</sub> Te	96-210-4349	0.7789
<b>and 150 others...</b>			

## Search-Match

### Settings

Reference database used COD-Inorg

REV81284 2013.04.15 Automatic zeropoint

adaptation Yes

Minimum figure-of-merit (FoM) 0.60

Parameter/influence 2theta 0.50

Parameter/influence intensities 0.50

Parameter multiple/single phase(s) 0.50



## Peak List

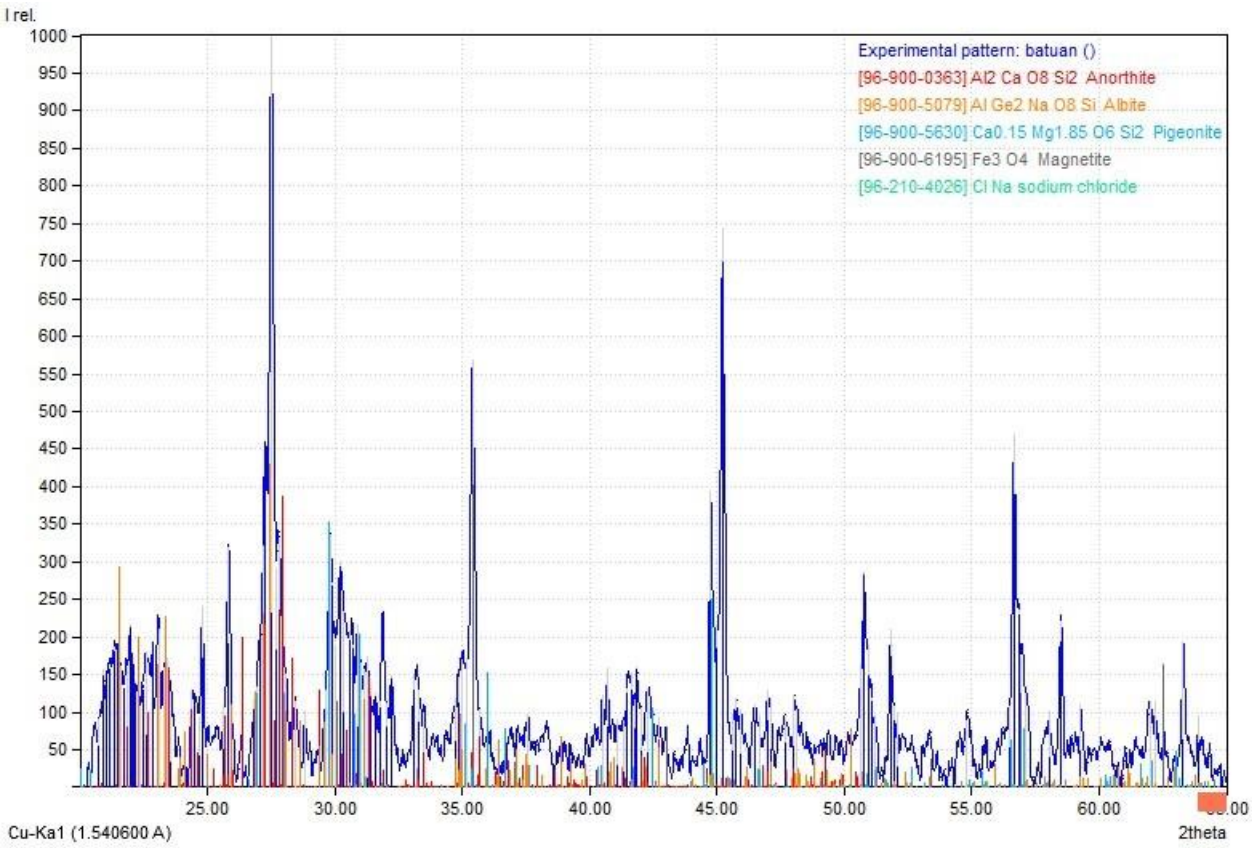
No.	2theta [°]	d [Å]	h/k/l	FWHM	Matched
1	20.75	4.2780	90.33	0.3200	A,C
2	20.93	4.2409	156.06	0.3200	A
3	21.05	4.2170	155.56	0.3200	
4	21.19	4.1900	156.18	0.3200	
5	21.34	4.1612	185.67	0.3200	A
6	21.47	4.1352	179.10	0.3200	
7	21.62	4.1078	161.24	0.3200	A,B
8	21.71	4.0903	130.99	0.3200	
9	21.85	4.0645	158.00	0.3200	A,C
10	21.96	4.0449	215.63	0.3200	A
11	22.07	4.0246	162.16	0.3200	
12	22.13	4.0142	132.09	0.3200	
13	22.19	4.0023	141.37	0.3200	A
14	22.35	3.9748	108.04	0.3200	A,B,C
15	22.50	3.9493	129.84	0.3200	
16	22.60	3.9316	180.46	0.3200	A
17	22.84	3.8911	192.42	0.3200	
18	23.11	3.8460	209.03	0.3200	A,B
19	23.28	3.8187	159.76	0.3200	A,B
20	23.41	3.7967	170.74	0.3200	A
21	23.57	3.7716	125.85	0.3200	A,B
22	24.38	3.6475	129.96	0.3200	A,B,C
23	24.49	3.6320	118.90	0.3200	

24	24.65	3.6085	93.36	0.3200	A
25	24.80	3.5876	239.22	0.3200	A,B,C
26	25.65	3.4707	107.07	0.3200	A,B
27	25.81	3.4487	317.83	0.3200	A
28	25.94	3.4316	107.67	0.3200	A,B
29	26.83	3.3204	115.17	0.3200	A,C
30	26.93	3.3083	132.84	0.3200	B,C
31	27.08	3.2905	206.47	0.3200	
32	27.18	3.2785	320.67	0.3200	A,B
33	27.25	3.2699	444.75	0.3200	
34	27.51	3.2398	1000.00	0.3200	A,B
35	27.69	3.2191	290.14	0.3200	A
36	27.83	3.2037	331.92	0.3200	A
37	27.95	3.1894	195.49	0.3200	A
38	28.09	3.1746	149.28	0.3200	A,B,C
39	28.43	3.1371	114.54	0.3200	A
40	28.83	3.0940	102.34	0.3200	A,B,C
41	29.65	3.0105	128.52	0.3200	A,B
42	29.82	2.9936	335.84	0.3200	A,C
43	29.89	2.9871	271.67	0.3200	A
44	30.05	2.9716	187.52	0.3200	B,D
45	30.19	2.9579	298.66	0.3200	A
46	30.35	2.9426	232.91	0.3200	A
47	30.57	2.9222	207.24	0.3200	A,C
48	30.71	2.9090	189.39	0.3200	A
49	30.88	2.8938	216.67	0.3200	A,B,C
50	31.01	2.8814	164.71	0.3200	B,C
51	31.15	2.8691	157.13	0.3200	A,B
52	31.28	2.8570	174.15	0.3200	A
53	31.39	2.8479	131.01	0.3200	A
54	31.59	2.8298	124.23	0.3200	A,B
55	31.79	2.8122	113.92	0.3200	A,B,C
56	32.02	2.7927	112.37	0.3200	A,C
57	32.23	2.7753	149.07	0.3200	A,B
58	33.13	2.7020	149.92	0.3200	A,B
59	33.29	2.6891	129.56	0.3200	A,B
60	33.51	2.6720	99.81	0.3200	A
61	34.71	2.5826	117.77	0.3200	A,B,C
62	34.87	2.5711	145.80	0.3200	A,B
63	35.01	2.5609	169.18	0.3200	A,B
64	35.17	2.5496	170.88	0.3200	A,B,C
65	35.40	2.5336	567.50	0.3200	A,C,D
66	35.68	2.5140	103.94	0.3200	A,B,C
67	37.59	2.3907	96.21	0.3200	A,B,C,D
68	40.50	2.2258	123.54	0.3200	A,B,C
69	40.69	2.2157	158.38	0.3200	A,B,C
70	41.09	2.1951	89.67	0.3200	A,B
71	41.35	2.1816	89.19	0.3200	A,B
72	41.48	2.1754	131.04	0.3200	C
73	41.65	2.1669	152.34	0.3200	A,B
74	41.75	2.1617	115.82	0.3200	B,C
75	41.87	2.1559	159.70	0.3200	A
76	42.01	2.1488	104.51	0.3200	A,B,C
77	42.25	2.1374	131.98	0.3200	A,B
78	42.47	2.1268	95.24	0.3200	A,B,C
79	42.69	2.1162	93.53	0.3200	A,B,C,D
80	44.76	2.0231	392.72	0.3200	A,B,C
81	45.01	2.0126	217.33	0.3200	A,B
82	45.22	2.0037	742.53	0.3200	A,B
83	45.62	1.9868	97.26	0.3200	A,B,C
84	45.73	1.9826	119.34	0.3200	A,C
85	45.93	1.9743	103.92	0.3200	A,B
86	46.52	1.9506	108.89	0.3200	A,C
87	46.66	1.9451	93.91	0.3200	A,B,C
88	46.99	1.9321	128.96	0.3200	A,B
89	47.10	1.9281	116.65	0.3200	A,B,C,D
90	47.67	1.9063	93.28	0.3200	A,B,C
91	48.03	1.8927	123.64	0.3200	A,B
92	48.13	1.8889	102.58	0.3200	A,B,C
93	50.65	1.8009	162.24	0.3200	A,B,C
94	50.79	1.7963	287.13	0.3200	A,B
95	50.92	1.7918	188.16	0.3200	A,C
96	51.07	1.7870	117.53	0.3200	A
97	51.19	1.7831	94.23	0.3200	A,B,C
98	51.81	1.7632	209.18	0.3200	B,C
99	51.93	1.7593	108.48	0.3200	B
100	52.08	1.7546	99.23	0.3200	B,C
101	54.81	1.6735	89.16	0.3200	B,C

102	56.47	1.6281	108.54	0.3200	B,C
103	56.66	1.6233	467.04	0.3200	B,C
104	56.85	1.6183	236.13	0.3200	B,C
105	56.95	1.6157	172.12	0.3200	C,D
106	57.11	1.6115	125.20	0.3200	B,C
107	58.03	1.5882	101.50	0.3200	B,C
108	58.48	1.5770	220.74	0.3200	B,C
109	59.26	1.5580	108.75	0.3200	B,C
110	61.99	1.4959	114.44	0.3200	B,C
111	62.20	1.4913	113.26	0.3200	B,D
112	63.29	1.4681	192.77	0.3200	B,C
113	63.90	1.4557	93.88	0.3200	B,C

Rietveld Refinement using FullProf

Diffraction Pattern Graphics



## Match! Phase Analysis Report

### Sample: S1#6A#2020

**Sample Data**  
File name S1#6A#2020.txt  
File path D:/Data/App kuliah/Macthnn/mahasiswa Geofisika(1)/mahasiswa Geofisika/S1#6A#2020  
Data collected Sep 7, 2020 15:04:20  
Data range 20.370° - 65.350°  
Number of points 2251  
Step size 0.020  
Rietveld refinement converged

No Alpha2 subtracted

Yes  
Background subtr. Yes  
Data smoothed Yes  
2theta correction 0.37°  
Radiation X-rays  
Wavelength 1.540598 Å

### Matched Phases

Index	Amount (%)	Name	Formula sum
A	43.6	Albite	Al Na O8 Si3
B	41.1	Pigeonite	Ca0.15 Mg1.85 O6 Si2
C	11.1	Diopside	Ca Mg O6 Si2
D	4.2	Periclase	Mg O

#### A: Albite (43.6 %)

Formula sum Al Na O8 Si3  
Entry number 96-900-1258  
Figure-of-Merit (FoM) 0.839164  
Total number of peaks 249  
Peaks in range 225  
Peaks matched 214  
Intensity scale factor 0.39  
Space group C -1  
Crystal system triclinic (anorthic)  
Unit cell a= 8.1370 Å b= 12.7850 Å c= 7.1583 Å  $\alpha$ = 94.260°  $\beta$ = 116.600°  $\gamma$ = 87.710°  
I/Icor 0.83  
Calc. density 2.623 g/cm<sup>3</sup>  
Reference Armbruster T., Burgi H. B., Kunz M., Gnos E., Bronnimann S., Lienert C.,  
"Variation of displacement parameters in structure refinements of low albite  
Note: this sample of feldspar is from Roc Tourne, France", American

Mineralogist **75**, 135-140 (1990)

**B: Pigeonite (41.1 %)**

Formula sum Ca<sub>0.15</sub> Mg<sub>1.85</sub> O<sub>6</sub> Si<sub>2</sub>  
Entry number 96-900-5630  
Figure-of-Merit (FoM) 0.851706  
Total number of peaks 437  
Peaks in range 143  
Peaks matched 131  
Intensity scale factor 0.43  
Space group P 1 2<sub>1</sub>/c 1  
Crystal system monoclinic  
Unit cell a= 9.6510 Å b= 8.8460 Å c= 5.2520 Å β= 108.380 °  
I/I<sub>cor</sub> 0.95  
Calc. density 3.169 g/cm<sup>3</sup>  
Reference Merli M., Camara F., "Topological analysis of the electron density of the clinopyroxene structure by the maximum entropy method: an exploratory study Sample: Dien2 Note: c-cell parameter changed by personal communication with author, Dec 2003", European Journal of Mineralogy **15**, 903-911 (2003)

**C: Diopside (11.1 %)**

Formula sum Ca Mg O<sub>6</sub> Si<sub>2</sub>  
Entry number 96-100-0010  
Figure-of-Merit (FoM) 0.820395  
Total number of peaks 221  
Peaks in range 73  
Peaks matched 72  
Intensity scale factor 0.15  
Space group C 1 2<sub>1</sub>/c 1  
Crystal system monoclinic  
Unit cell a= 9.6808 Å b= 8.8488 Å c= 5.2180 Å β= 105.606 °  
I/I<sub>cor</sub> 1.25  
Calc. density 3.341 g/cm<sup>3</sup>  
Reference Thompson R. M., Downs R. T., "The crystal structure of diopside at pressure to 10 GPa Locality: DeKalb, New York Sample: P = 2.32 GPa", American Mineralogist **93**, 177-186 (2008)

**D: Periclase (4.2 %)**

Formula sum Mg O  
Entry number 96-901-3209  
Figure-of-Merit (FoM) 0.819541  
Total number of peaks 9  
Peaks in range 2  
Peaks matched 2  
Intensity scale factor 0.16  
Space group F m -3 m  
Crystal system cubic  
Unit cell a= 3.9130 Å

I/Icor 3.13  
Calc. density 4.467 g/cm<sup>3</sup>  
Reference Jacobsen S. D., Holl C. M., Adams K. A., Fischer R. A., Martin E. S., Bina C. R., Lin J. F., Prakapenka V. B., Kubo A., Dera P., "Compression of single-crystal magnesium oxide to 118 GPa and a ruby pressure gauge for helium pressure media Note: P = 53.0 GPa using ruby-scale Note: P = 55.1 GPa using MgO-scale", *American Mineralogist* **93**, 1823-1828 (2008)

# Candidates

<b>Name</b>	<b>Formula</b>	<b>Entry No.</b>	<b>FoM</b>
Barium fluoroniobate *	Ba4 F12 Nb2 O3	96-100-0325	0.8048
	Ga6 O25 Sc4 Sr10	96-432-8033	0.8003
	Bi5.91 La2.1 Pb2 S14	96-431-9504	0.7987
	C6 Cl3 N3 O6	96-200-1647	0.7948
Calcium catena-polyphosphate	Ca O6 P2	96-400-1395	0.7940
Copper(I) copper zinc molybdat (1/1/1.75/3)	Cu2 Mo3 O12 Zn1.75	96-200-2671	0.7924
	Cr1.98 Er6.02 S11	96-430-1423	0.7880
	Ba5.4 Eu0.6 Ge25	96-810-0506	0.7879
	Bi5.42 La2.56 S14 Sr2	96-431-9505	0.7873
Holmium polysulfide	Ho6 S11.091	96-432-7786	0.7864
	Cs3 H4 O12 P S2	96-210-1352	0.7858
Galenobismutite	Bi0.91 Cl0.1 Pb0.575 S1.792 Se0.131	96-900-4983	0.7858
	C22 F14	96-411-2715	0.7839
	Cs2 Ga O10 P3	96-700-9289	0.7830
Tribarium hexafluoroaluminate trifluoride - Ib	Al Ba3 F9	96-100-0330	0.7826
Cupromakovickyite	Ag0.52 Bi4.48 Cu2 Pb S9	96-901-0667	0.7813
Dibarium copper(I) dioxide iodide	Ba2 Cu I O2	96-200-2478	0.7806
Nonacalcium octachloride bis(dicarbidoborate)	B2 Ca9 Cl8	96-100-5054	0.7800
Lanthanum strontium copper oxide (0.8/1.2/1/3.4)	Cu La0.74 O4 Sr1.2	96-100-1205	0.7792
	Fe2 S11 Yb6	96-201-0166	0.7780
	Ga3.25 La12 Sb24.02	96-810-3053	0.7771
Galenobismutite	Bi1.85 Cl0.168 Pb1.14 S3.738 Se0.094	96-900-4982	0.7769
	N2 O4 Si2 Sr3	96-432-8643	0.7761
praseodymium gallium antimonide	Ga3.98 Pr12 Sb22.9	96-432-1411	0.7728
Monoclinic titanium metaphosphate	O27 P9 Ti3	96-201-0156	0.7725
Lillianite	Bi2 Pb3 S6	96-900-9251	0.7721
	C Ba3 F7 O3 Sc	96-201-0336	0.7717
Tribarium scandium carbonate heptafluoride	Ba3 F7 O3 Sc	96-100-0362	0.7716
Galenobismutite	Bi2 Pb S3.87 Se0.13	96-900-4976	0.7716
	Al Cs 2 O10 P3	96-700-9288	0.7711
	Ca2 Co0.9 O7 Si2 Zn0.1	96-210-0542	0.7710
	Ca2 Co0.9 O7 Si2 Zn0.1	96-901-1317	0.7710
Beryllium	Be	96-901-2021	0.7710
Marialite	C0.24 Al3.56 Ca1.24 Cl0.76 Na2.76 O28 Si8.44	96-901-3342	0.7707
caesium copper(I) silver(I) cyanide, CsAgCu(CN)3	C9 Ag3 Cs3 Cu3 N9	96-410-4977	0.7695
Silver divanadate	Ag4 O7 V2	96-100-7101	0.7694
alpha-Zn4Sb3	Sb10 Zn13	96-411-3279	0.7694
Pentaprasedymiumtrisiliconnonanitride	N9 Pr5 Si3	96-222-2175	0.7693
Terbium polysulfide	S10.945 Tb6	96-432-7788	0.7692
PotassiumDihydrogenPhosphate	H2 K O4 P	96-702-0837	0.7688
Braunite	Fe2.38 Mn11.62 O24 Si	96-900-0775	0.7688
Dysprosium polysulfide	Dy6 S11.144	96-432-7789	0.7686
Leucite	Al O6 Rb Si2	96-900-1797	0.7684
Nonastrontium tetrazinc dicopper(I) oxide	Cu2 O14 Sr9 Zn4	96-200-2521	0.7683
Beryllium	Be	96-901-2022	0.7683
	Ca13 Mg5 Na18 O72 P18	96-901-1517	0.7681
Clinokurchatovite	B2 Ca Mg O5	96-901-1895	0.7677
Cerium triiodate	Ce I3 O9	96-201-4794	0.7675
	Ca2 Co0.9 O7 Si2 Zn0.1	96-210-0541	0.7675
	Ca2 Co0.9 O7 Si2 Zn0.1	96-901-1316	0.7675
Marialite	C0.24 Al3.56 Ca1.24 Cl0.76 Na2.76 O28 Si8.44	96-901-3344	0.7670
Trivanadium(III) silicopentaphosphate	O19 P5 Si V3	96-100-1684	0.7667

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## Settings

Reference database used COD-Inorg

REV81284 2013.04.15 Automatic zeropoint

adaptation Yes

Minimum figure-of-merit (FoM) 0.60

Parameter/influence 2theta 0.50

Parameter/influence intensities 0.50

Parameter multiple/single phase(s) 0.50

## Peak List

<b>No.</b>	<b>2theta [°]</b>	<b>d [Å]</b>	<b>I/I0</b>	<b>FWHM</b>	<b>Matched</b>
1	20.69	4.2901	57.25	0.4398	A,B,C
2	21.80	4.0737	254.08	0.4398	A,B
3	22.49	3.9499	24.06	0.4398	B
4	23.02	3.8606	131.70	0.4398	A
5	23.96	3.7118	265.44	0.4398	A,B,C
6	24.96	3.5651	228.88	0.4398	A,B
7	25.20	3.5307	226.81	0.4398	
8	25.53	3.4858	261.27	0.4398	A
9	25.67	3.4681	261.08	0.4398	
10	25.91	3.4354	270.68	0.4398	A
11	26.05	3.4180	279.53	0.4398	
12	26.19	3.3993	297.37	0.4398	A,B,C
13	28.05	3.1785	1000.00	0.4398	A,B,C
14	28.83	3.0944	104.04	0.4398	A
15	29.40	3.0358	6.66	0.4398	B
16	30.25	2.9518	724.58	0.4398	A,B,C
17	30.85	2.8957	515.16	0.4398	A,B,C
18	31.56	2.8328	294.69	0.4398	A,B,C
19	32.39	2.7619	187.16	0.4398	A,B
20	33.70	2.6573	148.98	0.4398	A
21	34.43	2.6028	77.32	0.4398	A,B
22	35.27	2.5429	316.34	0.4398	A,B,C

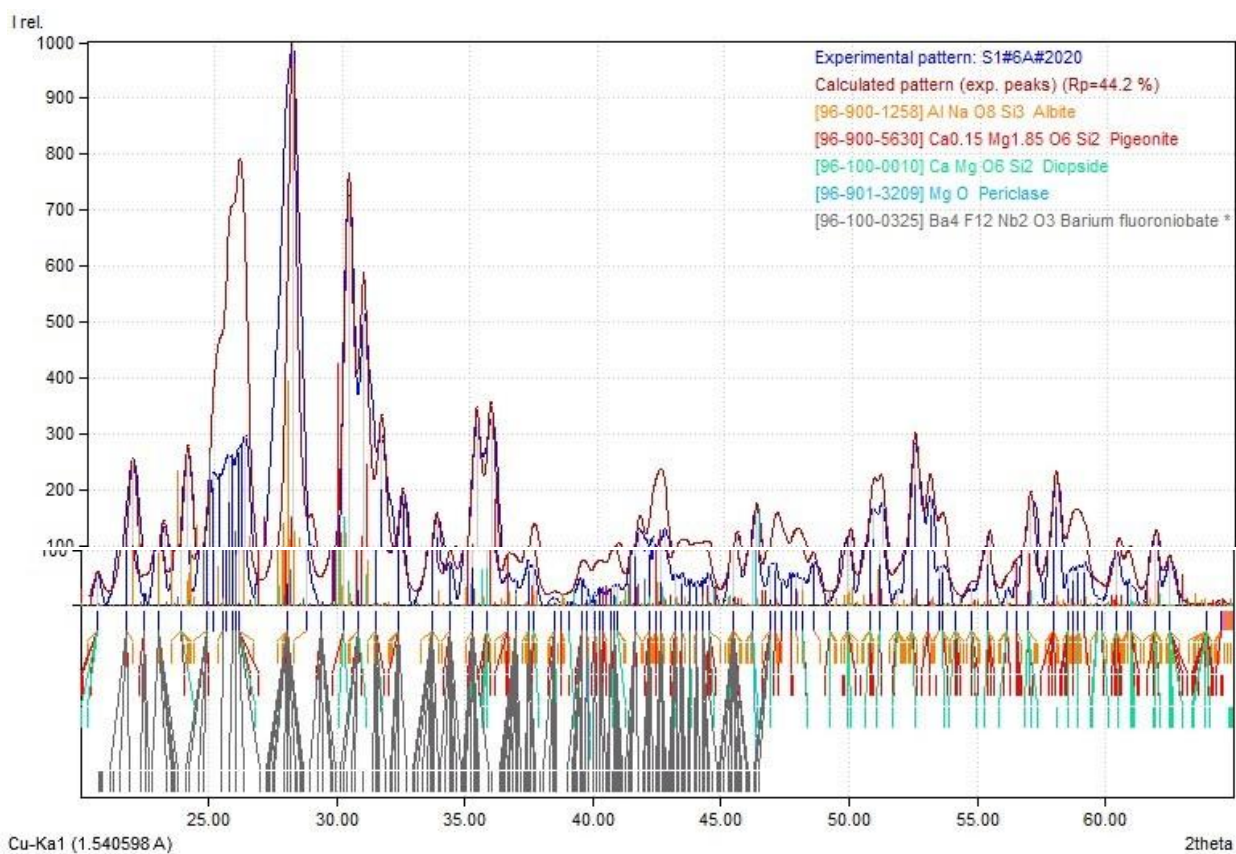


23	35.85	2.5030	327.53	0.4398	A,B,C
24	36.69	2.4475	59.06	0.4398	A,B
25	36.99	2.4283	49.52	0.4398	A
26	37.47	2.3981	79.92	0.4398	A
27	37.66	2.3865	72.03	0.4398	A,B,C
28	38.49	2.3373	15.10	0.4398	A,B,C
29	38.76	2.3215	7.03	0.4398	A,B
30	39.05	2.3045	8.11	0.4398	C
31	39.54	2.2774	50.57	0.4398	A,B
32	39.74	2.2661	35.64	0.4398	A,D
33	40.08	2.2479	22.89	0.4398	A,B
34	40.26	2.2385	32.37	0.4398	
35	40.40	2.2306	24.08	0.4398	A,B
36	40.71	2.2147	32.67	0.4398	C
37	40.85	2.2075	37.66	0.4398	B,C
38	40.98	2.2005	38.14	0.4398	A,C
39	41.66	2.1661	128.73	0.4398	A,B
40	42.18	2.1406	114.58	0.4398	A,B,C
41	42.44	2.1282	109.88	0.4398	A,B
42	42.64	2.1185	128.89	0.4398	A,B,C
43	43.22	2.0914	58.38	0.4398	A,B,C
44	43.49	2.0794	57.00	0.4398	A,B
45	43.80	2.0654	49.10	0.4398	C
46	44.05	2.0540	44.92	0.4398	A,B
47	44.29	2.0433	48.21	0.4398	B
48	44.52	2.0334	58.53	0.4398	A,B,C
49	45.50	1.9921	115.17	0.4398	A,B,C
50	46.26	1.9611	162.24	0.4398	A,B,C,D
51	46.94	1.9343	75.06	0.4398	A,B,C
52	47.12	1.9273	78.56	0.4398	A,B
53	47.38	1.9173	47.62	0.4398	B
54	47.73	1.9038	62.21	0.4398	B
55	47.94	1.8960	57.83	0.4398	A
56	48.18	1.8874	51.00	0.4398	A,B,C
57	48.63	1.8708	78.60	0.4398	A
58	49.24	1.8492	10.33	0.4398	A,B,C
59	49.94	1.8248	121.07	0.4398	A,B,C
60	50.81	1.7954	168.52	0.4398	A,B,C
61	51.17	1.7838	175.58	0.4398	A,B,C
62	51.88	1.7609	30.29	0.4398	A,B,C
63	52.47	1.7426	280.73	0.4398	A,B,C
64	53.06	1.7245	187.39	0.4398	A,B
65	53.50	1.7113	70.37	0.4398	A
66	53.66	1.7067	73.60	0.4398	A,B,C
67	54.13	1.6929	3.40	0.4398	A,B,C
68	54.78	1.6743	30.63	0.4398	A,B,C
69	55.37	1.6578	120.28	0.4398	A,B,C
70	56.19	1.6358	31.01	0.4398	A,B,C
71	56.51	1.6271	45.41	0.4398	A,B
72	57.00	1.6144	184.32	0.4398	A,B,C
73	57.98	1.5893	218.54	0.4398	A,B
74	58.54	1.5755	58.95	0.4398	A,B,C
75	58.72	1.5710	68.65	0.4398	A,B
76	58.93	1.5659	72.93	0.4398	A,C
77	59.20	1.5596	80.33	0.4398	A,B
78	59.66	1.5485	17.19	0.4398	A,C
79	59.87	1.5435	11.11	0.4398	A,B,C
80	60.46	1.5301	96.71	0.4398	A,B,C
81	60.89	1.5202	47.76	0.4398	A
82	61.00	1.5176	37.37	0.4398	A,B,C
83	61.91	1.4976	120.52	0.4398	A,B,C
84	62.53	1.4843	80.49	0.4398	A,B,C
85	63.92	1.4553	2.88	0.4398	A,B,C
86	64.53	1.4430	9.12	0.4398	A,B

### Rietveld Refinement using FullProf

Calculation was not run or did not converge.

### Diffraction Pattern Graphics



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