

Phase Analysis Report

Hasanuddin University

Sample: serbuk ()

Sample Data

File name	hx#bu#anti.RAW
File path	C:/Users/lenovo/Desktop/2021 Kirim Data/04 admin 6 Agustus 2021/bu anti
	XRD XRF/hx#bu#anti
Data collected	Aug 7, 2021 10:44:48
Data range	15.070° - 70.070°
Number of points	2751
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	0.07°
Radiation	X-rays
Wavelength	1.540600 Å

Matched Phases

Index	Amount (%)	Name	Formula sum
A	97.2	Hydroxylapatite	Ca ₅ H ₂ O ₁₃ P ₃
B	2.8	Calcium	Ca

A: Hydroxylapatite (97.2 %)

Formula sum	Ca ₅ H ₂ O ₁₃ P ₃
Entry number	96-900-2215
Figure-of-Merit (FoM)	0.850377
Total number of peaks	134
Peaks in range	62
Peaks matched	43
Intensity scale factor	0.98
Space group	P 6 ₃ /m
Crystal system	hexagonal
Unit cell	a= 9.4394 Å c= 6.8861 Å
I/I _{cor}	1.63
Calc. density	3.145 g/cm ³
Reference	Wilson R. M., Elliot J. C., Dowker S. E. P., "Rietveld refinement of the crystallographic structure of human dental enamel apatites Sample: H6G, synthetic", American Mineralogist 84 , 1406-1414 (1999)

B: Calcium (2.8 %)

Formula sum	Ca
Entry number	96-901-1035
Figure-of-Merit (FoM)	0.749823
Total number of peaks	9
Peaks in range	5
Peaks matched	4
Intensity scale factor	0.22
Space group	I m -3 m
Crystal system	cubic
Unit cell	a= 4.4800 Å
I/I _{cor}	10.07
Calc. density	1.479 g/cm ³
Reference	Bernstein B. T., Smith J. F., "Coefficients of thermal expansion for face-

centered cubic and body-centered cubic calcium Locality: synthetic Sample: at
T = 467 C", Acta Crystallographica **12**, 419-420 (1959)

Candidates

Name	Formula	Entry No.	FoM
Alkaline-earth Apatite	Ca10 Cu H O26 P6	96-700-1907	0.8652
Fluorapatite	Ca4.961 F O12 P3 Th0.039	96-901-3551	0.8637
Apatite-(CaF)	Ca4.961 F O12 P3 Th0.039	96-901-3556	0.8637
Fluorapatite	Ca4.584 Dy0.258 F Na0.158 O12 P2.874 Si0.12	96-900-1675	0.8629
Fluorapatite	C0.042 Ca5 F0.921 O12.321 P2.883	96-901-0505	0.8568
Calcium tris(phosphate) fluoride (Fluorapatite)	Ca10 F2 O24 P6.05	96-500-0042	0.8564
Fluorapatite	C0.078 Ca5 F0.842 O12.402 P2.895	96-901-0506	0.8557
Fluorapatite	Ca4.791 F0.93 Mn0.211 O12 P3	96-900-1391	0.8552
Fluorapatite	Ca5 F O12 P3	96-210-4745	0.8541
Fluorapatite	Ca5 F O12 P3	96-210-4756	0.8540
Fluorapatite	Ca4.958 F O12 P3 U0.042	96-901-3549	0.8498
Apatite-(CaF)	Ca4.958 F O12 P3 U0.042	96-901-3554	0.8498
Fluorapatite	C0.066 Ca5 F0.864 O12.381 P2.883	96-901-0507	0.8490
Carbonate-hydroxylapatite	C0.26 Ca5 O13.686 P2.829	96-900-3551	0.8489
Carbonate-hydroxylapatite	C0.26 Ca5 O13.686 P2.829	96-900-3555	0.8489
Hydroxylapatite-dental	Ca4.73 H1.58 Mg0.02 Na0.1 O11.73 P2.79	96-900-2222	0.8477
Hydroxylapatite-dental	Ca4.73 H1.16 Mg0.05 Na0.1 O11.88 P2.76	96-900-2218	0.8458
Calcium fluoride tris(phosphate) (Fluorapatite)	Ca5 F O12 P3	96-101-1045	0.8456
Hydroxylapatite-dental	Ca4.73 H1.1 Mg0.02 Na0.1 O12.36 P2.85	96-900-2228	0.8455
Carbonate-hydroxylapatite	C0.22 Ca5 O13.514 P2.823	96-900-3552	0.8454
Carbonate-hydroxylapatite	C0.22 Ca5 O13.514 P2.823	96-900-3556	0.8454
Pentacalcium tris(phosphate) fluoride (Fluorapatite)	Ca5 F O12 P3	96-101-0997	0.8452
Hydroxylapatite-dental	Ca4.7 H1.24 Mg0.02 Na0.1 O12.2 P2.73	96-900-2223	0.8448
Fluorapatite	Ca5 F O12 P3	96-900-6955	0.8416
Hydroxylapatite	Ca4.557 Ce0.423 F0.335 H2 Na0.02 O12.664 P2.595 Si0.405	96-900-1344	0.8413
Alkaline-earth Apatite	Ca10 Cu H O26 P6	96-700-1908	0.8377
Chlorapatite	Ca4.899 Cl La0.052 Na0.05 O12 P3	96-900-2435	0.8377
Pentacalcium tris(phosphate) hydroxide (Hydroxylapatite)	Ca5 H O13 P3	96-101-1243	0.8356
Carbonate-fluorapatite	Ca2.108 F0.171 O8.817 P1.362	96-900-9981	0.8318
Fluorapatite	Ca5 F O12 P3	96-900-6954	0.8306
Hydroxylapatite	As0.33 Ca5 H O13 P2.67	96-901-3629	0.8293
Oxyapatite	Ho7.73 Na2.27 O24.72 Si6	96-222-1593	0.8266
Hydroxylapatite-dental	Ca4.73 H1.76 Mg0.02 Na0.1 O11.81 P2.79	96-900-2221	0.8229
Hydroxylapatite-dental	Ca4.73 H1.46 Mg0.02 Na0.1 O12.85 P2.76	96-900-2227	0.8228
Carbonate-fluorapatite	Ca2.07 F0.163 O8.922 P1.239	96-900-9980	0.8222
Hydroxylapatite-dental	Ca4.76 H1.62 Mg0.02 Na0.1 O12.25 P2.82	96-900-2225	0.8220
Hydroxylapatite	Ca5 H2 O13 P3	96-900-2215	0.8215
Apatite-(CaOH)	Ca5 H2 O13 P3	96-901-0051	0.8215
Hydroxylapatite-dental	Ca4.76 H1.78 Mg0.02 Na0.1 O12.04 P2.85	96-900-2224	0.8204
Hydroxylapatite-dental	Ca4.7 H2 Mg0.02 Na0.1 O12.09 P2.76	96-900-2229	0.8201
Fluorapatite	Ca5 Cl0.33 F0.39 H2 O12.28 P3	96-900-1263	0.8185
Carbonate-fluorapatite	Ca2.019 F0.165 O8.832 P1.182	96-900-9979	0.8158
Chlorapatite	Ca4.822 Cl2 Na0.087 Nd0.092 O12 P3	96-900-2433	0.7988
chlorapatite	Ca5 Cl O12 P3	96-210-5263	0.7987
chlorapatite	Ca5 Cl O12 P3	96-210-5264	0.7985
Chlorapatite	Ca4.857 Cl2 Dy0.069 Na0.072 O12 P3	96-900-2434	0.7983
chlorapatite	Ca5 Cl O12 P3	96-210-5262	0.7978
Chlorapatite	Ca4.899 Cl2 La0.052 Na0.05 O12 P3	96-900-2432	0.7970
Barium As-apatite	As3 Ba5 Cl O12	96-221-9457	0.7945
chlorapatite	Ca5 Cl O12 P3	96-210-5265	0.7934
chlorapatite	Ca5 Cl O12 P3	96-210-5266	0.7876

Hydroxylapatite
and 6 others...

As_{0.727} Ca₅ H O₁₃ P_{2.273}

96-901-3630 0.7869

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

Selection Criteria

Compound:

Name: apatite

Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	15.83	5.5934	67.09	0.0400	
2	16.17	5.4770	115.11	0.0400	
3	16.23	5.4556	72.62	0.0400	
4	16.35	5.4178	72.90	0.0400	
5	16.55	5.3521	96.75	0.0400	
6	16.65	5.3196	75.46	0.0400	
7	16.79	5.2758	147.91	0.0400	A
8	16.93	5.2344	127.86	0.0400	
9	17.09	5.1842	121.38	0.0400	
10	17.13	5.1720	162.43	0.0400	
11	17.25	5.1373	114.39	0.0400	
12	17.35	5.1071	78.53	0.0400	
13	17.49	5.0669	122.72	0.0400	
14	17.73	4.9975	83.97	0.0400	
15	17.90	4.9514	134.30	0.0400	
16	18.06	4.9079	72.86	0.0400	
17	18.17	4.8784	81.61	0.0400	
18	18.28	4.8493	123.48	0.0400	
19	18.41	4.8156	105.93	0.0400	
20	18.53	4.7850	94.74	0.0400	
21	18.69	4.7428	136.52	0.0400	
22	18.83	4.7081	105.36	0.0400	A
23	18.93	4.6830	119.59	0.0400	
24	19.04	4.6584	133.69	0.0400	
25	19.15	4.6309	95.21	0.0400	
26	19.25	4.6071	135.35	0.0400	
27	19.49	4.5519	83.89	0.0400	
28	19.67	4.5089	110.67	0.0400	
29	19.81	4.4781	77.91	0.0400	
30	19.95	4.4479	123.90	0.0400	
31	20.07	4.4204	123.71	0.0400	
32	20.23	4.3871	103.54	0.0400	
33	20.50	4.3296	108.98	0.0400	
34	20.64	4.2999	114.74	0.0400	
35	20.95	4.2364	72.96	0.0400	
36	21.17	4.1931	77.62	0.0400	

37	21.28	4.1724	89.83	0.0400	
38	21.55	4.1197	80.40	0.0400	
39	21.81	4.0718	143.32	0.0400	
40	21.93	4.0497	109.06	0.0400	
41	22.17	4.0064	145.73	0.0400	
42	22.33	3.9778	91.22	0.0400	
43	22.44	3.9588	76.88	0.0400	
44	22.77	3.9022	86.05	0.0400	A
45	22.93	3.8752	103.96	0.0400	
46	23.10	3.8467	82.25	0.0400	
47	23.35	3.8066	79.76	0.0400	
48	23.77	3.7401	62.76	0.0400	
49	23.95	3.7128	74.50	0.0400	
50	25.62	3.4742	100.63	0.0400	
51	25.69	3.4649	186.06	0.0400	
52	25.75	3.4564	278.10	0.0400	
53	25.85	3.4433	633.23	0.0400	A
54	25.91	3.4360	843.69	0.0400	
55	26.01	3.4228	889.74	0.0400	
56	26.07	3.4154	745.07	0.0400	
57	26.23	3.3951	304.51	0.0400	
58	26.27	3.3896	245.36	0.0400	
59	26.39	3.3746	113.96	0.0400	
60	28.01	3.1828	125.95	0.0400	
61	28.13	3.1699	159.45	0.0400	A,B
62	28.19	3.1634	232.11	0.0400	
63	28.39	3.1416	154.27	0.0400	
64	28.51	3.1282	122.07	0.0400	
65	28.77	3.1006	77.57	0.0400	
66	28.90	3.0865	203.39	0.0400	A
67	29.09	3.0676	197.96	0.0400	
68	29.19	3.0569	178.87	0.0400	
69	29.31	3.0450	140.19	0.0400	
70	29.61	3.0148	63.28	0.0400	
71	31.12	2.8716	86.91	0.0400	
72	31.24	2.8608	94.45	0.0400	
73	31.35	2.8511	193.79	0.0400	
74	31.49	2.8383	280.23	0.0400	
75	31.60	2.8292	386.13	0.0400	
76	31.67	2.8230	478.74	0.0400	
77	31.76	2.8152	683.15	0.0400	A
78	31.87	2.8054	795.73	0.0400	
79	31.93	2.8008	1000.00	0.0400	
80	32.08	2.7883	935.10	0.0400	A
81	32.31	2.7685	883.93	0.0400	
82	32.45	2.7569	582.20	0.0400	
83	32.51	2.7515	536.51	0.0400	
84	32.62	2.7427	451.68	0.0400	
85	32.69	2.7368	366.51	0.0400	
86	32.85	2.7244	551.53	0.0400	A
87	32.91	2.7197	657.08	0.0400	
88	33.00	2.7122	716.80	0.0400	
89	33.09	2.7048	763.25	0.0400	
90	33.28	2.6897	612.96	0.0400	
91	33.39	2.6814	481.90	0.0400	
92	33.63	2.6625	141.00	0.0400	
93	33.79	2.6504	115.40	0.0400	
94	34.03	2.6327	188.76	0.0400	A
95	34.16	2.6224	274.83	0.0400	
96	34.36	2.6076	216.41	0.0400	
97	34.51	2.5967	203.77	0.0400	
98	34.67	2.5853	125.42	0.0400	

99	34.84	2.5734	119.39	0.0400	
100	34.95	2.5654	100.05	0.0400	
101	35.11	2.5537	80.83	0.0400	
102	35.23	2.5454	81.20	0.0400	
103	35.37	2.5359	75.03	0.0400	A
104	35.55	2.5230	115.00	0.0400	
105	35.77	2.5084	102.42	0.0400	
106	35.91	2.4990	96.19	0.0400	
107	36.09	2.4870	76.88	0.0400	
108	36.29	2.4734	70.74	0.0400	
109	39.27	2.2924	87.17	0.0400	
110	39.61	2.2735	146.41	0.0400	
111	39.77	2.2644	264.80	0.0400	A
112	39.95	2.2552	350.28	0.0400	
113	40.11	2.2465	297.64	0.0400	
114	40.23	2.2399	264.73	0.0400	B
115	40.34	2.2340	205.51	0.0400	A
116	40.45	2.2283	126.55	0.0400	
117	40.61	2.2196	100.18	0.0400	
118	40.75	2.2125	67.24	0.0400	A
119	40.87	2.2062	80.34	0.0400	
120	41.64	2.1672	66.69	0.0400	
121	41.77	2.1606	79.76	0.0400	
122	41.91	2.1539	73.07	0.0400	A
123	42.19	2.1402	105.71	0.0400	
124	42.31	2.1344	85.87	0.0400	A
125	42.47	2.1267	144.91	0.0400	
126	43.12	2.0962	65.33	0.0400	
127	43.71	2.0694	77.81	0.0400	
128	43.93	2.0596	97.29	0.0400	
129	44.04	2.0547	176.10	0.0400	
130	44.17	2.0487	83.85	0.0400	
131	44.73	2.0245	63.44	0.0400	
132	45.21	2.0039	62.87	0.0400	A
133	45.43	1.9948	121.80	0.0400	
134	45.57	1.9889	82.17	0.0400	
135	45.84	1.9781	68.72	0.0400	
136	46.48	1.9520	100.88	0.0400	
137	46.59	1.9478	120.51	0.0400	A
138	46.71	1.9429	219.04	0.0400	
139	46.84	1.9378	343.87	0.0400	
140	46.99	1.9323	271.39	0.0400	
141	47.11	1.9275	218.66	0.0400	
142	47.23	1.9230	133.05	0.0400	
143	47.33	1.9191	80.35	0.0400	
144	47.57	1.9098	73.57	0.0400	
145	47.91	1.8971	93.05	0.0400	
146	48.07	1.8913	125.83	0.0400	A
147	48.18	1.8871	158.65	0.0400	
148	48.42	1.8783	197.98	0.0400	
149	48.57	1.8730	171.61	0.0400	A
150	48.73	1.8671	112.35	0.0400	
151	48.84	1.8632	118.89	0.0400	
152	49.05	1.8558	72.78	0.0400	
153	49.33	1.8459	138.51	0.0400	
154	49.48	1.8406	276.62	0.0400	A
155	49.63	1.8354	355.54	0.0400	
156	49.69	1.8334	322.66	0.0400	
157	49.87	1.8272	171.40	0.0400	B
158	49.98	1.8232	197.74	0.0400	
159	50.18	1.8166	85.98	0.0400	
160	50.34	1.8113	138.65	0.0400	A

161	50.51	1.8055	184.77	0.0400	
162	50.67	1.8000	204.59	0.0400	
163	50.81	1.7955	184.95	0.0400	
164	50.96	1.7904	139.02	0.0400	
165	51.11	1.7857	178.60	0.0400	
166	51.21	1.7823	132.64	0.0400	A
167	51.37	1.7772	178.83	0.0400	
168	51.56	1.7710	172.44	0.0400	
169	51.73	1.7656	172.61	0.0400	
170	51.90	1.7602	80.73	0.0400	
171	52.06	1.7554	107.20	0.0400	A
172	52.33	1.7469	179.88	0.0400	
173	52.51	1.7414	107.76	0.0400	
174	52.65	1.7370	75.05	0.0400	
175	53.04	1.7252	95.28	0.0400	A
176	53.21	1.7200	378.34	0.0400	A
177	53.40	1.7145	398.31	0.0400	
178	53.55	1.7098	260.40	0.0400	
179	53.83	1.7018	96.34	0.0400	
180	53.98	1.6973	70.21	0.0400	
181	55.83	1.6453	85.23	0.0400	A
182	55.97	1.6417	72.16	0.0400	
183	56.09	1.6385	72.22	0.0400	
184	56.19	1.6356	78.84	0.0400	A
185	56.32	1.6322	72.31	0.0400	
186	57.18	1.6096	85.51	0.0400	
187	57.40	1.6039	65.75	0.0400	
188	58.37	1.5797	85.40	0.0400	
189	58.94	1.5658	72.29	0.0400	
190	59.81	1.5450	78.93	0.0400	A
191	59.97	1.5413	111.81	0.0400	
192	60.13	1.5375	131.53	0.0400	
193	60.24	1.5350	138.10	0.0400	A
194	60.39	1.5316	131.51	0.0400	
195	60.53	1.5283	118.33	0.0400	
196	60.80	1.5223	72.25	0.0400	
197	61.46	1.5075	85.27	0.0400	A
198	61.58	1.5049	72.09	0.0400	A
199	61.73	1.5015	124.67	0.0400	
200	61.83	1.4993	111.49	0.0400	
201	61.95	1.4967	104.89	0.0400	
202	62.06	1.4943	144.33	0.0400	
203	62.41	1.4868	65.32	0.0400	
204	62.77	1.4791	71.83	0.0400	
205	62.91	1.4761	91.54	0.0400	A
206	63.05	1.4732	111.25	0.0400	
207	63.19	1.4702	117.81	0.0400	
208	63.35	1.4669	111.21	0.0400	A
209	63.47	1.4644	98.05	0.0400	
210	63.59	1.4620	111.19	0.0400	
211	63.72	1.4593	78.30	0.0400	
212	63.91	1.4555	117.77	0.0400	A
213	64.03	1.4531	157.23	0.0400	A
214	64.19	1.4498	157.24	0.0400	
215	64.35	1.4466	137.52	0.0400	
216	64.63	1.4410	84.94	0.0400	
217	64.79	1.4378	84.97	0.0400	
218	64.95	1.4346	131.04	0.0400	A
219	65.13	1.4311	150.81	0.0400	A
220	65.25	1.4288	124.52	0.0400	
221	65.39	1.4261	131.13	0.0400	
222	65.51	1.4237	118.00	0.0400	

223	65.84	1.4174	72.05	0.0400	B
224	66.31	1.4085	98.46	0.0400	A
225	69.53	1.3510	72.75	0.0400	A
226	69.63	1.3492	62.38	0.0400	

Rietveld Refinement using FullProf

Diffraction Pattern Graphics