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The crystal structure of viitaniemiite

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Abstract

The crystal structure of viitaniemiite $Na(Ca,Mn)AlPO_4F_2OH$ $a = 5.457(2)$, $b = 7.151(2)$, $c = 6.836(2)$Å, $\beta = 109.36(3)°$ $V = 251.68$Å^3, $Z = 2$, space gro P2$_1$/m, has been solved by Patterson and Fourier methods and refined by the least-squ es method to an R index of 0.037 for 728 observed ($>2\sigma$) reflections. The structure con as two sets of infinite chains parallel to the b-axis, one composed of $AlO_2(OH)_2F_2$ octahedra sharing opposite OH corners and the other of $(Ca,Mn)O_4F_2$ octahedra sharing opposite O–O edges. These chains alternate laterally sharing F corners to form a set of parallel sheets held together by PO_4 tetrahedra and NaO_4F_4 gable disphenoids.

The sheet structure of viitaniemiite containing octahedrally coordinated atoms in two separate positions resembles that of montebrasite and eosphorite. These three related phosphate minerals are associated with each other in the type locality of viitaniemiite, Viitaniemi pegmatite, Orivesi, southern Finland, where they crystallized during hydrothermal replacement processes caused by residual fluids of the pegmatite melt.

Introduction

Viitaniemiite occurs as a rare hydrothermal mineral in the phosphate-rich Viitaniemi pegmatite, Orivesi, southern Finland. One of the authors (SIL) has described it as a new mineral in a study on the mineralogy and petrology of the granitic pegmatities of the Eräjärvi area (Lahti, 1981). The mineral was encountered as an inclusion in eosphorite aggregate and is associated with morinite, another aluminum-bearing phosphate mineral. Structure analysis confirmed the ideal formula $Na(Ca,Mn)AlPO_4F_2OH$ with $Z = 2$, although wet chemical analysis indicates that some of the fluorine may be replaced by OH groups. The crystal data measured during the structure analysis are given in Table 1. The X-ray powder data, the optical properties, the chemical data, and the mineralogical description of the mineral have been given by Lahti (1981) and are not reproduced here. A preliminary description of the structure has been given by Lahti and Pajunen (1982). To date viitaniemiite has been identified positively in only three localities: at Viitaniemi, in museum specimens collected from druses of granite in Greifenstein, Sachsen (East Germany), and from Francon quarry, northeastern Montreal, where its occurrence has been confirmed by Ramik et al. (1983). In this quarry viitaniemiite was encountered as very small crystals in vesicles of silicocarbonatite together with cryolite, calcite, quartz, and weloganite. Because the powder diffraction data of viitaniemiite resemble those of an unnamed mineral from Greifenstein, Sachsen, given on JCPDS card 13-0587, the present authors studied several museum specimens taken from this locality and identified viitaniemiite from the samples labeled as lacroixite (cf. Mrose, 1971). According to the descriptins by Slavik (1914, 1915), lacroixite (and therefore also viitaniemiite) occurs there in druses of lithiogranite together with ježekite (sodian morinite), apatite, childrenite (Fe end member of the isomorphous series childrenite-eosphorite), roscherite, and tourmaline. Preliminary microanalyzer determinations showed that Greifenstein viitaniemiite is rich in calcium and contains only a few percent of manganese; the fluorine content, however, is equal to that of the Finnish viitaniemiite. Due to its different chemical composition, the Greifenstein viitaniemiite has a larger unit cell ($a = 5.48$Å, $b = 7.18$Å, $c = 6.85$Å, $\beta = 109.00°$, $V = 254.84$Å^3; based on the precession films from sample no. 86746 in Harvard Mineralogical Museum). Detailed studies on the Greifenstein viitaniemiite and lacroixite are in progress, because some of the data cited for lacroixite obviously derive from viitaniemiite.

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ITANIEMITE NA(CA,MN)ALPO4F2OH

0,0,L

1	115	-98
2	667	622
3	411	-372
4	400	371
5	65	-54
6	369	361
7	233	-232
8	321	324
9	116	-120

0,1,L

1	190	-185
2	389	382
3	172	157
4	166	158
5	187	186
6	93	-95
7	79	76
8	38	39

0,2,L

0	219	205
1	152	149
2	97	-78
3	397	-394
4	357	349
5	29	28
6	268	270
7	164	172
8	112	118

0,3,L

1	184	-169
2	394	-377
3	81	76
4	41	-36
5	249	-257
6	28	24
7	30	-29

0,4,L

0	1119	1089
1	88	-75
2	610	603
3	143	-132
4	157	156
5	90	-94
6	344	346
7	146	-145
8	241	255

0,5,L

1	145	-146
2	211	211
3	80	88
4	106	107
5	116	117
6	84	-84
7	59	58

0,6,L

0	20	-15
1	34	32
2	206	199
3	187	-184
4	189	184
5	62	-62
6	249	251
7	148	158

0,7,L

1	49	50
2	173	-170
3	16	-13
4	42	-45
5	99	-105
6	66	64

0,8,L

0	464	453
1	60	-58
2	316	319
3	32	-34
4	61	58
5	59	-65

0,9,L

2	129	128
3	49	-45

0,10,L

0	63	63

1,0,L

-9	165	170
-8	185	185
-7	69	61
-6	235	-235
-5	202	205
-4	191	-185
-3	613	606
-2	137	-135
-1	271	276
0	133	139
1	286	272
2	561	-537
3	543	524
4	92	-91
5	514	505
6	94	-89
7	26	29
8	50	-53

1,1,L

-9	120	120
-8	35	33
-7	55	-53
-6	202	203
-4	23	28
-3	44	53
-2	320	-305
-1	165	166
0	54	58
1	289	-303
2	108	112
3	44	-51
4	42	-33
5	89	82
6	145	-148
8	40	39

1,2,L

-9	298	300
-8	114	-113
-7	384	373
-6	201	-197
-5	263	248
-4	169	166
-3	749	671
-1	871	851
0	364	-379
1	405	432
2	212	-196
3	249	258
4	264	286
5	347	351
6	72	-72
7	191	203
8	110	-116

1,3,L

-8	66	-62
-7	37	-40
-6	173	-164
-5	158	151
-3	284	-256
-2	175	159
-1	148	120
0	81	81
1	48	53
2	241	-238
3	161	162
4	125	133
5	114	-120
6	48	53

1,4,L

-8	95	94
-7	89	86
-6	105	-99
-5	200	183
-4	316	-293
-3	452	431
-2	101	91
-1	294	276
0	115	-112
1	89	86
2	221	-231
3	500	517
4	131	-133
5	298	326
6	57	-60
7	70	75

1,5,L

-8	37	27
-7	69	-70
-6	150	147
-4	31	28
-3	42	30
-2	184	-175
-1	104	107
0	43	42
1	200	-208
2	82	88
3	24	-18
5	56	56
6	128	-124

1,6,L

-7	309	297
-6	36	-41
-5	164	156
-3	351	327
-2	127	130
-1	529	523
0	316	-314
1	206	206
2	16	-7
3	221	239
4	109	120
5	166	175
6	46	-42

1,7,L

-6	132	-126
-5	43	41
-3	44	-43
-2	124	119
-1	49	-54
0	42	-37
1	127	125
2	81	-84
3	57	57
5	73	-73

1,8,L

-5	150	141
-4	212	-201
-3	255	249
-2	60	61
-1	158	161
0	43	-42
1	81	74
2	80	-82
3	302	316
4	106	-113

1,9,L

-3	94	94
-2	74	-72
-1	41	-32
1	43	-40
2	124	124
3	40	-44

2,0,L

-9	101	-103
-8	257	263
-7	151	-150
-6	85	84
-5	184	197
-4	408	417
-3	352	368
-2	169	202
-1	290	-304
0	693	721
1	511	513
2	453	440
3	220	214
4	56	49
5	50	-42
6	150	142
7	148	-148

2,1,L

-9	89	87
-8	31	22
-7	154	-151
-6	66	75
-5	125	-120
-4	125	-127
-3	69	-58
-2	347	-370
-1	43	45
0	211	217
1	101	-102
2	240	237
3	90	93
4	68	69
5	175	181
6	53	-53

2,2,L

-9	20	-17
-8	144	146
-7	48	-51
-6	372	363
-5	195	-193
-4	822	805
-3	341	-324
-2	155	160
-1	641	-653
0	216	217
1	192	-197
2	632	642
3	321	-333
4	431	441
5	144	-150
6	188	193
7	33	32

2,3,L

-8	26	-27
-7	42	41
-6	108	-104
-5	246	247
-4	203	199
-3	139	-132
-2	128	124
-1	94	91
0	31	31
1	29	35
2	336	-349
3	77	-76
4	39	37
5	155	-153
7	26	-16

2,4,L

-8	171	165
-7	148	-142
-6	183	176
-5	199	188
-4	203	192
-3	134	137
-2	343	334
-1	85	-79
0	453	468
1	153	164
2	343	358
3	237	252
4	57	60
5	93	-96
6	116	116
7	98	-101

2,5,L

-8	25	23
-7	128	-126
-6	67	67
-5	66	-62
-4	72	-67
-3	32	-32
-2	248	-243
-1	55	54
0	157	156
1	85	-94
2	126	141
3	50	53
4	49	47
5	132	134
6	48	-48

2,6,L

-7	51	-46
-6	345	339
-5	91	-85
-4	407	394
-3	249	-244
-2	214	205
-1	138	-137
0	67	64
1	172	-183
2	385	402
3	124	-127
4	282	304
5	142	-155
6	121	130

2,7,L

-6	65	-65
-5	84	86
-4	72	66
-3	39	-31
-2	143	138
-1	18	-16
0	65	-60
1	71	70
2	125	-124
3	49	-41
5	112	-113

2,8,L

-5	98	94
-4	91	83
-3	23	25
-2	231	232
-1	57	-58
0	258	263
1	25	18
2	207	212
3	136	141
4	46	48

2,9,L

-4	74	-72
-3	65	54
-2	71	-69
1	30	-36
2	131	136

3,0,L

-9	107	115
-8	63	65
-7	325	339
-6	221	-235
-5	306	309
-4	463	-491
-3	307	321
-2	246	-245
-1	220	219
0	152	155
1	540	535
2	224	-215
3	25[illegible]	244
4	1[illegible]	-180
5	241	240
6	122	117
7	80	72

3,1,L

-9	108	110
-8	109	115
-7	56	-56
-6	153	157
-5	34	35
-3	94	99
-2	269	-275
-1	75	-80
0	65	65
1	206	-214
2	20	21
3	19	-24
4	78	-70
5	123	117
6	64	-63
7	31	-24

3,2,L

-9	154	150
-8	52	-48
-7	348	344
-6	143	145
-5	153	152
-4	149	152
-3	326	334
-2	56	-56
-1	592	620
0	14	14
1	423	439
2	49	-52
4	57	-55
5	281	278
6	41	-47

3,3,L

-9	38	-38
-8	56	-52
-6	227	-224
-5	39	38
-4	132	138
-3	147	-148
-2	78	83
-1	86	84
0	83	83
1	193	201
2	126	-128
4	123	122
5	70	-73
6	34	28

3,4,L

-7	229	226
-6	129	-127
-5	355	349
-4	411	-411
-3	146	145
-2	125	-120
-1	285	284
0	110	125
1	306	309
2	191	-193
3	268	279
4	125	-122
5	172	174
6	64	66

3,5,L

-8	104	101
-7	54	-53
-6	102	100
-5	33	23
-3	79	81
-2	198	-199
-1	20	-19
0	61	64
1	145	-152
4	36	-41
5	109	107

3,6,L

-7	207	202
-6	142	139
-5	188	187
-4	44	47
-3	133	123
-2	37	-37
-1	486	492
0	32	-33
1	186	193
2	40	-46
3	69	70
5	174	174

3,7,L

-6	95	-94
-5	20	-11
-4	34	33
-3	71	-75
-2	140	137
-1	33	34
0	29	-32
1	90	98
2	46	-46
3	19	8
4	56	55

3,8,L

-5	246	241
-4	237	-236
-3	94	92
-2	36	-36
-1	181	179
0	58	62
1	156	168
2	108	-113

3,9,L

-2	47	-44
0	27	-27

4,0,L

-9	143	-146
-8	344	360
-7	67	-66
-6	136	139
-5	132	-139
-4	312	326
-3	109	107
-2	753	772
-1	273	-275
0	442	444
1	118	-118
2	292	280
3	39	35
4	256	248
5	99	-91
6	233	223

4,1,L

-9	41	45
-8	69	67
-7	117	-119
-6	22	21
-5	46	-38
-4	104	-109
-3	110	114
-2	178	-181
-1	21	-23
0	149	150
1	34	-35
2	107	103
3	92	86
4	38	-36
5	138	129

4,2,L

-9	63	60
-8	124	121
-7	47	25
-6	182	183
-5	245	-244
-4	283	283
-3	106	117
-2	154	157
-1	26	38
0	79	-80
1	137	-139
2	219	214
3	63	-61
4	243	240
5	88	90

4,3,L

-8	19	8
-7	78	74
-6	126	-124
-5	41	38
-4	213	222
-3	79	-78
-2	51	53
-1	40	-36
0	57	-56
1	85	91
2	120	-124
3	119	-117
4	54	53
5	99	-96

VITTANIEMIITE NA(CA,MN)ALPO4F2OH

4,4,L

-8	280	278
-7	126	-128
-6	129	129
-5	43	-13
-4	257	252
-2	538	551
-1	138	-139
0	387	397
1	123	-128
2	180	181
3	53	54
4	234	238
5	84	-86

4,5,L

-7	99	-93
-4	60	-61
-3	97	96
-2	141	-146
-1	27	-29
0	119	120
1	37	-38
2	73	74
3	58	57
4	29	-22

4,6,L

-7	66	-62
-6	177	171
-5	96	-88
-4	229	230
-3	25	-27
-2	93	94
-1	90	97
0	24	25
1	141	-144
2	131	135
3	40	-41

4,7,L

-6	41	-39
-4	87	88

-3	70	-69
-2	90	93
-1	24	7
0	71	-68
1	43	41
2	49	-51

4,8,L

-4	143	136
-3	57	-50
-2	301	302
-1	75	-75
0	238	241
1	76	-86

5,0,L

-7	139	143
-6	95	-98
-5	215	217
-4	142	-137
-3	119	119
-1	41	-46
0	34	-30
1	346	339
3	317	292
4	105	-93

5,1,L

-8	132	138
-7	30	-26
-6	87	88
-5	37	41
-4	77	-82
-3	104	102
-2	152	-148
-1	120	-124
0	30	38
1	118	-119
3	29	25
4	73	-68

5,2,L

-8	181	-184

-7	255	258
-6	74	76
-5	278	278
-4	97	100
-3	405	412
-2	179	-178
-1	308	305
0	143	-138
1	233	233
2	106	100
3	101	93
4	74	-70

5,3,L

-8	60	-61
-7	48	45
-6	155	-150
-5	65	-66
-4	140	140
-3	42	-42
-2	76	75
-1	61	61
1	166	163
3	59	-56
4	55	55

5,4,L

-7	71	70
-6	113	-112
-5	258	253
-4	83	-79
-3	63	65
-2	59	-54
0	22	22
1	279	274
2	35	-36
3	253	251

5,5,L

-7	29	-23
-6	62	61
-5	29	26
-4	51	-54
-3	80	80

-2	120	-118
-1	98	-94
0	53	51
1	77	-81

5,6,L

-6	30	27
-5	244	245
-4	94	95
-3	234	232
-2	176	-174
-1	252	251
0	64	-63
1	152	149
2	28	29

5,7,L

-4	58	56
-3	60	-58
-2	62	62
-1	78	77
0	28	-27

6,0,L

-8	179	183
-7	97	102
-6	145	143
-5	62	59
-4	38	37
-3	52	-51
-2	321	309
-1	30	23
0	208	202
1	85	85
2	26	22
3	35	24

6,1,L

-8	86	90
-7	78	-74
-6	36	34
-4	72	-75
-3	94	97

-2	19	-14
-1	70	-67
0	114	108
1	51	-50
2	55	43
3	56	52

6,2,L

-7	42	-43
-6	307	307
-5	211	-208
-4	161	161
-3	111	-100
-2	156	148
-1	25	23
0	215	215
1	152	-141
2	223	211

6,3,L

-7	115	111
-6	74	-71
-5	61	-61
-4	92	92
-3	29	-33
-1	23	23
0	109	-100
1	70	71
2	30	-28

6,4,L

-6	86	82
-5	68	66
-4	82	80
-3	61	-65
-2	229	225
0	214	206
1	80	74

6,5,L

-4	59	-53
-3	79	77
-1	66	-64

0	88	86

6,6,L

-3	79	-76
-2	72	70

7,0,L

-6	196	-193
-5	181	171
-4	154	-142
-3	133	129
-2	46	47
-1	114	103
0	110	-101

7,1,L

-6	48	46
-5	37	34
-4	87	-80
-3	43	37
-2	32	-32
-1	116	-107
0	25	33

7,2,L

-6	95	92
-5	72	70
-4	66	60
-3	258	250
-1	186	173
0	70	-65

7,3,L

-5	73	-70
-4	74	73
-2	47	38
-1	82	74

7,4,L

-3	130	120