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The crystal structure of vuagnatite, $CaAl(OH)SiO_4$

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Abstract

The new orthorhombic mineral vuagnatite, $CaAl(OH)SiO_4$ ($P2_12_12_1$, a = 7.055(6), b = 8.542(7), c = 5.683(5)Å, Z = 4) is isotypic with conichalcite, $CaCu(OH)AsO_4$. From counter diffractometer data corrected for absorption [$\mu(MoK\alpha)$ = 22.5cm^{-1}] the structure was refined anisotropically to a final R value of 0.043 for 974 reflections ($F > 3\sigma$). Vuagnatite is characterized by $AlO_4(OH)_2$ octahedra sharing edges to form chains linked by isolated SiO_4 tetrahedra and CaO_7OH polyhedra. The Donnay-Allmann empirical method of recognizing O^{2-}, $(OH)^-$, and H_2O in crystal structures indicates the presence of only one hydroxyl group, creating a hydrogen bond between the tetrahedral oxygen O(2) and the octahedral oxygen O(5). The position of the hydrogen atom was confirmed from a difference Fourier synthesis and successfully refined. The bond distance O(5)–H (the hydroxyl group) is 0.94(5)Å and the O(2)–O(5) distance is 2.530(3)Å with a value of 178(6)° for the angle O(2)···H–O(5). Two oxygen atoms of each AlO_6 octahedron are hydroxyl groups. The crystal chemical formula of vuagnatite is therefore $Ca^{[8]}Al^{[6]}(OH)Si^{[4]}O_4$.

Introduction

Vuagnatite, $CaAl(OH)SiO_4$, is a new silicate mineral found in a metasomatic rodingite from Bögürtlencik Tepe in southwest Turkey. Its mineralogical data have been reported in the preceding article (Sarp *et al.*, 1976). This paper reports its crystal structure, with particular emphasis on determining the role of hydrogen, since by classical methods it was impossible in this material to quantify either the total water content or its role as $(OH)^-$ or H_2O.

Experimental

Single crystals from crushed rock samples (containing predominantly hydrogarnet and chlorite (clinochlore) and minor amounts of prehnite and vesuvianite) were isolated and oriented for X-ray study by their optical ellipsoids on a spindle stage. Reciprocal-lattice explorer and Weissenberg films of four crystals indicated an orthorhombic unit cell. Systematic absences of the type h odd for $h00$, k odd for $0k0$ and l odd for $00l$ lead uniquely to space group $P2_12_12_1$.

Intensities of an anhedral crystal (approximately 0.14 × 0.10 × 0.06 mm) were measured on a Philips PW1100 computer-controlled four-circle diffractometer using $MoK\alpha$ radiation (λ = 0.71069Å), graphite monochromator, in the $\theta/2\theta$ scan mode. Data were collected in one octant of reciprocal space from θ = 3 to 38°. A total of 1084 nonequivalent reflections was measured out to sin θ/λ = 0.866Å^{-1} of which 974 had F_{obs} greater than 3σ. Absorption correction was applied to the data using the program CAMEL JOCKEY (Flack 1974, 1975). For this, eight families of eight equivalent planes were additionally measured using the ψ scan method. The least-squares refinement, using the program LATTIX (Gvildys, 1965), of $1/d$ values of 23 families of parallel planes yielded the following cell parameters (e.s.d.'s at the 3σ level): a = 7.055(6), b = 8.542(7), c = 5.683(5) Å.

Structure solution and refinement

Chemical formula, space group, and axial ratios a/b and c/b suggest an isotypy to the conichalcite [$CaCu(OH)AsO_4$] structure studied by Qurashi and Barnes (1963). The calculated powder pattern based on conichalcite atomic positions shows a close fit to the observed powder intensities[2] (Table 3, Sarp *et al.*,

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[2] Close also to those of a sample from Japan (A. Kato, 1975, private communication).

TABLE 7. Vuagnatite. Observed and calculated structure factors*

H,0,0

h	L	$10F_{obs.}$	$10F_{calc.}$
2		454	478
4		808	840
6		242	253
8		552	572
10		116	125
12		170	167
14		81	75
16		76	67
18		32	24

H,1,0

h	L	$10F_{obs.}$	$10F_{calc.}$
1		193	198
2		97	102
3	L	20	20
4		72	81
5		459	482
6		151	159
7		170	177
8		85	85
9		53	47
10		33	40
11		140	134
12		139	133

H,2,0

h	L	$10F_{obs.}$	$10F_{calc.}$
0		139	111
1		64	58
2		295	294
3		454	460
4		856	893
5		169	174
6		364	378
7		224	228
8		183	185
9		31	38
10	L	0	15
11		177	172
12		170	163

H,3,0

h	L	$10F_{obs.}$	$10F_{calc.}$
1		792	808
2		840	851
3		130	132
4		59	56
5		129	128
6		125	123
7		358	369
8		125	134
9		341	345
10		93	87
11	L	0	6

H,4,0

h	L	$10F_{obs.}$	$10F_{calc.}$
0		153	148
1		596	551
2		277	287
3		244	240
4		362	370
5		238	243
6		213	215
7		165	166
8		74	73
9		100	103
10	L	29	32
11		61	76

H,5,0

h	L	$10F_{obs.}$	$10F_{calc.}$
1		174	154
2		34	35
3		585	605
4		174	182
5		320	326
6		223	222
7	L	35	24
8		282	279
9		34	7
10		67	66
11		102	104

H,6,0

h	L	$10F_{obs.}$	$10F_{calc.}$
0		698	605
1		152	140
2		295	290
3	L	29	3
4		238	249
5		185	182
6		39	18
7	L	0	5
8		453	451
9		79	84
10		211	207
11	L	0	3

H,7,0

h	L	$10F_{obs.}$	$10F_{calc.}$
1		66	41
2	L	55	7
3		528	539
4		125	122
5		324	324
6	L	38	35
7		77	80
8		122	114
9	L	47	15
10	L	0	11

H,8,0

h	L	$10F_{obs.}$	$10F_{calc.}$
0		627	534
1		204	178
2		221	209
3		141	138
4		609	619
5		148	154
6		43	34
7		155	158
8		116	118
9	L	0	4
10		114	114

H,9,0

h	L	$10F_{obs.}$	$10F_{calc.}$
1		542	476
2		275	256
3		114	119
4	L	37	35
5		161	164
6		266	265
7		123	119
8	L	30	31
9		314	302

H,10,0

h	L	$10F_{obs.}$	$10F_{calc.}$
0		236	195
1	L	48	33
2		124	126
3		129	124
4		71	68
5		128	121
6		146	140

* Table of The Crystal Structure of Vuagnatite $CaAl(OH)SiO_4$, Mc NEAR, E., M.G. VINCENT and E. PARTHE (1976) Am. Mineral.
The columns are h, L (less than 3σ), $10F_{obs.}$ and $10F_{calc.}$
The scale factor is $F_{obs.} \times 2.140(6) = F_{rel.}$ (shift/error: 0.009).

H,10,0

h	$10F_o$	$10F_c$
7	86	87
8	116	122

H,11,0

h	$10F_o$	$10F_c$
1 L	0	21
2	590	529
3	266	250
4 L	0	12
5	272	266
6	281	277
7 L	0	10
8 L	0	21

H,12,0

h	$10F_o$	$10F_c$
0	374	305
1 L	54	25
2	153	137
3	131	126
4	50	9
5	66	52
6 L	36	52
7	69	68

H,13,0

h	$10F_o$	$10F_c$
1	61	62
2	151	123
3 L	0	18
4	117	103
5	178	169

H,14,0

h	$10F_o$	$10F_c$
0	163	129

H,16,0

h	$10F_o$	$10F_c$
0	182	143

H,18,0

h	$10F_o$	$10F_c$
0	123	109

H,0,1

h	$10F_o$	$10F_c$
1	40	33
2	939	978
3	124	122
4	62	59
5	44	41
6	730	762
7	143	150
8	125	128
9	142	144
10	298	303
11 L	31	3
12 L	0	6

H,1,1

h	$10F_o$	$10F_c$
0	51	24
1	296	287
2	160	159
3	160	166
4	162	164
5	194	203
6	200	202
7	197	199
8	133	133
9	56	61
10	179	181
11	140	131
12	58	52

H,2,1

h	$10F_o$	$10F_c$
0	171	165
1 L	59	39
2	599	611
3	214	213
4	64	67
5	193	193
6	193	196
7	116	115
8	41	32
9	148	148
10	155	155
11	198	194
12	94	90

H,3,1

h	$10F_o$	$10F_c$
0 L	0	16
1	602	641
2	102	100
3	594	605
4	327	334
5	319	329
6	151	159
7	353	361
8	195	199
9	176	177
10	56	51
11	203	203

H,4,1

h	$10F_o$	$10F_c$
0	46	29
1	289	287
2	177	188
3	137	140
4	137	131
5	188	189
6	181	185
7	109	106
8	84	84
9	138	144
10	120	114
11	77	63

H,5,1

h	$10F_o$	$10F_c$
0	472	406
1	334	326
2	124	133
3	373	391
4	111	108
5	210	208
6	120	118
7	197	201
8	130	123
9	211	207
10	176	171
11	115	113

H,6,1

h	$10F_o$	$10F_c$
0	122	102
1	265	249
2	565	589
3	155	161
4	94	94
5	156	153
6	251	248
7	203	200

H,6,1

h	$10F_o$	$10F_c$
8	75	82
9	111	112
10	182	178
11	132	129

H,7,1

h	$10F_o$	$10F_c$
0	91	70
1	67	65
2	102	105
3	220	239
4	94	100
5	108	108
6	116	114
7	92	96
8 L	30	33
9	62	63
10	133	122

H,8,1

h	$10F_o$	$10F_c$
0 L	49	39
1	275	247
2	360	349
3	122	131
4 L	0	34
5	272	274
6	379	377
7	92	93
8	53	48
9	165	171
10	173	172

H,9,1

h	$10F_o$	$10F_c$
0	380	319
1	257	225
2	93	85
3	187	192
4	169	180
5	126	137
6	101	103
7	234	236
8	113	118
9	40	49

H,10,1

h	$10F_o$	$10F_c$
0 L	42	55
1 L	39	66
2 L	46	27
3	100	95
4	58	49
5	79	76
6	61	53
7	74	78
8	74	82

H,11,1

h	$10F_o$	$10F_c$
0	343	278
1	260	214
2	103	87
3	172	166
4	342	342
5	149	143
6	69	82
7	98	105
8	267	257

H,12,1

h	$10F_o$	$10F_c$
0 L	0	20
1	89	70
2	173	147
3	169	142
4	100	103
5	78	89
6	158	166
7	57	48

H,13,1

h	$10F_o$	$10F_c$
0	175	147
1 L	0	10
2 L	50	39
3	78	72
4	100	96
5	107	102

H,0,2

h	$10F_o$	$10F_c$
0	782	761
1 L	47	5
2	404	393
3	111	107
4	786	792
5	130	134
6	112	110
7	31	14
8	111	114
9	111	112
10	82	74
11	52	56

H,1,2

h	$10F_o$	$10F_c$
0	129	113
1	731	688
2	676	638
3	410	402
4	173	172
5	124	125
6	129	131
7	232	234
8	133	135
9	284	291
10	52	50
11	43	44

H,2,2

h	$10F_o$	$10F_c$
0	126	148
1	361	321
2	402	398
3	101	105
4	135	131
5	282	287
6	184	186
7	131	129
8	312	316
9	88	85
10	140	136
11	144	134

H,3,2

h	$10F_o$	$10F_c$
0	202	195
1	498	469
2	300	292
3	932	940
4	158	161
5	728	741
6 L	25	24
7	142	146
8	148	148
9	187	189

H,3,2

h		$10F_o$	$10F_c$
10		50	42
11		160	153

H,4,2

h		$10F_o$	$10F_c$
0		701	685
1		48	50
2		420	412
3		139	143
4		126	122
5		69	71
6		114	113
7		35	12
8		208	208
9		165	162
10		189	183
11	L	40	14

H,5,2

h		$10F_o$	$10F_c$
0	L	31	28
1		798	820
2		47	45
3		347	341
4		160	160
5		133	128
6		151	150
7		394	394
8		176	177
9		259	261
10		91	94
11		69	67

H,6,2

h		$10F_o$	$10F_c$
0	L	35	37
1		417	437
2		158	161
3		253	262
4		527	534
5		311	312
6		357	359
7		156	160
8		167	166
9		103	105
10		91	85

H,7,2

h		$10F_o$	$10F_c$
0		169	145
1		225	229
2		147	153
3		120	123
4		88	89
5		202	208
6		97	101
7		144	136
8		103	110
9		81	76
10	L	34	28

H,8,2

h		$10F_o$	$10F_c$
9		741	645
1		312	299
2		181	190
3		284	300
4		100	97
5		156	159
6		206	212
7		212	210
8		199	204
9		42	41

H,9,2

h		$10F_o$	$10F_c$
0		95	81
1		56	22
2	L	0	13
3		185	186
4		75	93
5		315	324
6		138	135
7		62	66
8		77	82
9		95	96

H,10,2

h		$10F_o$	$10F_c$
0		386	334
1	L	44	43
2		193	190
3		[illegible]	144
4	L	[illegible]	26
5		[illegible]	125
6		94	94
7		[illegible]	[illegible]
8		116	127

H,11,2

h		$10F_o$	$10F_c$
0		58	10
1		333	301
2		329	323
3		89	56
4	L	37	26
5		68	61
6		120	129
7		237	231

H,12,2

h		$10F_o$	$10F_c$
0		229	187
1		116	84
2		63	82
3		137	127
4		312	316
5		77	80
6		155	152

H,13,2

h		$10F_o$	$10F_c$
0	L	53	32
1		86	77
2	L	44	32
3		270	254
4		72	81
5	L	48	32

H,0,3

h		$10F_o$	$10F_c$
1		249	245
2		668	651
3		237	229
4		92	92
5		54	53
6		520	520
7		99	100
8		38	36
9		166	163
10		291	285
11		125	122

H,1,3

h		$10F_o$	$10F_c$
0		125	116
1		416	389

h	$10F_o$	$10F_c$
	H,1,3	
2	113	111
3	150	147
4	129	123
5	232	231
6	170	165
7	128	130
8	108	102
9	139	139
10	119	125
11	102	101
	H,2,3	
0	396	363
1	47	52
2	343	331
3	99	[illegible]
4	185	184
5	177	176
6	181	177
7	179	179
8	115	117
9	111	112
10	96	95
11	156	151
	H,3,3	
0	63	70
1	563	515
2	144	145
3	516	508
4	233	229
5	306	311
6 L	27	8
7	315	316
8	170	165
9	178	176
10	91	98
11	198	195
	H,4,3	
0	230	212
1	106	102
2	197	187
3	152	148
4	257	254
5	142	140
6	137	138
7	162	162
8	185	184
9	104	106
10	52	57
11	36	16
	H,5,3	
0	201	200
1	304	296
2	61	49
3	357	355
4	96	96
5	274	275
6	134	132
7	225	226
8	192	198
9	176	179
10	165	168
	H,6,3	
0 L	0	12
1	252	254
2	443	434
3	222	219
4	62	56
5	165	165
6	217	217
7	177	184
8	86	83
9	89	87
10	158	158
	H,7,3	
0	72	71
1	155	156
2	57	61
3	90	85
4	157	152
5	81	76
6	209	204
7	100	100
8	67	71
9	107	105
10	95	95
	H,8,3	
0	108	108
1	190	209
2	277	287
3	130	130
4	176	184
5	238	236
6	313	310
7 L	31	56
8	65	59
9	163	158
	H,9,3	
0	252	230
1	162	161
2	107	100
3	157	159
4	159	164
5	84	82
6	39	44
7	156	154
8	68	78
	H,10,3	
0	303	265
1	88	88
2	113	121
3	74	83
4	83	98
5	60	63
6	52	51
7	126	124
8	135	124
	H,11,3	
0	260	223
1	183	173
2	60	62
3	142	147
4	242	261
5	157	154
6	64	65
7	87	94

h		$10F_o$	$10F_c$
H,12,3			
0	L	0	3
1		161	143
2		174	168
3		179	185
4		133	143
5		54	50
6		128	138
H,13,3			
0		112	92
1		58	42
2		134	127
3	L	0	10
4	L	0	47
H,0,4			
0		1351	1382
1		67	64
2		174	177
3		175	171
4		529	533
5		187	191
6		211	204
7	L	28	3
8		453	449
9		108	111
10		113	117
11	L	0	27
H,1,4			
0		58	51
1		344	338
2		146	143
3		294	286
4		85	87
5		399	393
6		114	116
7		252	258
8		104	103
9		48	56
10		121	118
11		139	128
H,2,4			
0		119	121

h		$10F_o$	$10F_c$
1		167	157
2		294	279
3		173	163
4		561	556
5		88	84
6		335	339
7		199	198
8		147	149
9		65	73
10		73	73
11		102	107
H,3,4			
0		176	168
1		603	560
2		430	415
3		95	98
4		192	196
5		65	73
6		207	211
7		283	281
8		74	80
9		244	243
10		94	91
H,4,4			
0		171	164
1		323	301
2		381	361
3		167	170
4		285	276
5		108	110
6		207	208
7		57	59
8		67	72
9		96	106
10		143	138
H,5,4			
0		132	122
1		175	167
2		132	128
3		454	447
4		180	181
5		227	229
6		97	94
7		75	69

h		$10F_o$	$10F_c$
8		179	172
9		58	60
10		85	83
H,6,4			
0		542	495
1		203	201
2		287	286
3		87	84
4		123	123
5		160	166
6		38	36
7	L	33	34
8		326	326
9		116	108
H,7,4			
0		216	211
1		140	134
2		109	110
3		357	361
4		89	89
5		231	230
6		55	44
7		157	156
8		123	122
9	L	0	38
H,8,4			
0		316	312
1		122	120
2		290	291
3		90	95
4		522	519
5		97	98
6		105	106
7		91	88
8		122	124
H,9,4			
0		66	65
1		291	293
2		220	220
3		73	81
4		168	166

H,9,4

h		$10F_o$	$10F_c$
5		127	125
6		187	190
7		107	102
8		52	65

H,10,4

h		$10F_o$	$10F_c$
0		210	200
1		125	122
2		178	189
3		78	84
4		66	51
5		112	119
6		185	190
7		102	104

H,11,4

h		$10F_o$	$10F_c$
0	L	44	25
1	L	0	46
2		358	382
3		193	204
4		45	44
5		210	216
6		249	250

H,12,4

h		$10F_o$	$10F_c$
0		218	201
1		82	82
2		99	99
3		110	120
4		55	34
5		157	149

H,13,4

h		$10F_o$	$10F_c$
0		136	112
1		122	111
2		83	89
3		72	77

H,0,5

h		$10F_o$	$10F_c$
1		113	118
2		549	553
3		173	171
4		105	103
5	L	0	12
6		408	404
7		177	175
8		49	21
9		123	118
10		238	237

H,1,5

h		$10F_o$	$10F_c$
0		91	102
1		292	294
2		156	154
3		247	242
4		172	165
5		161	166
6		92	86
7		134	137
8		74	62
9		110	102
10		139	137

H,2,5

h		$10F_o$	$10F_c$
0		312	310
1		95	94
2		330	322
3		112	105
4		170	175
5		98	93
6		206	206
7		115	116
8		133	142
9		64	64
10		110	122

H,3,5

h		$10F_o$	$10F_c$
0		211	201
1		271	254
2		174	172
3		246	242
4		158	156
5		218	218
6		200	206
7		228	226
8		169	171
9		102	98
10		72	66

H,4,5

h		$10F_o$	$10F_c$
0		231	211
1		105	99
2		88	73
3		127	123
4		294	287
5		130	133
6		121	119
7	L	33	25
8		126	126
9		119	122

H,5,5

h		$10F_o$	$10F_c$
0		75	75
1		242	219
2		60	57
3		204	197
4		70	60
5		249	244
6		63	73
7		142	142
8		42	45
9		212	214

H,6,5

h		$10F_o$	$10F_c$
0		93	89
1		74	66
2		294	283
3		137	135
4		54	37
5		119	121
6		200	205
7		245	245
8		92	95
9		98	99

H,7,5

h		$10F_o$	$10F_c$
0	L	41	26
1		172	171
2		188	185
3		208	213
4	L	32	43
5		186	193
6		117	122
7		134	147
8		79	64

H,8,5

h	$10F_o$	$10F_c$
0	156	163
1	101	96
2	287	287
3	73	86
4	105	112
5	164	162
6	201	205
7	71	69
8	123	122

H,9,5

h	$10F_o$	$10F_c$
0	183	184
1	164	171
2	191	188
3	137	142
4	186	190
5 L	0	51
6	158	157
7	128	136

H,10,5

h	$10F_o$	$10F_c$
0	94	96
1	147	139
2 L	0	37
3	134	133
4	122	120
5	60	66
6	67	80

H,11,5

h	$10F_o$	$10F_c$
0	260	260
1	219	220
2	111	111
3	106	110
4	209	205
5	133	120

H,12,5

h	$10F_o$	$10F_c$
0 L	0	5
1	126	127
2	43	49
3	102	110

H,0,6

h	$10F_o$	$10F_c$
0	91	93
1	158	165
2	304	308
3 L	26	18
4	447	451
5	175	175
6	51	53
7 L	0	13
8	46	44
9	192	191

H,1,6

h	$10F_o$	$10F_c$
0 L	29	14
1	276	277
2	123	127
3	247	244
4	132	133
5	153	154
6	85	86
7	217	214
8	95	79
9	225	219

H,2,6

h	$10F_o$	$10F_c$
0	237	238
1	185	188
2	371	372
3	71	78
4	132	131
5	170	168
6	233	228
7	114	112
8	193	195
9	112	115

H,3,6

h	$10F_o$	$10F_c$
0	208	211
1	157	156
2	140	131
3	451	444
4	171	172
5	363	363
6	88	90
7	90	87
8	126	118
9	89	68

H,4,6

h	$10F_o$	$10F_c$
0	295	289
1 L	47	32
2	365	351
3	134	121
4	117	122
5	150	151
6	205	215
7	124	117
8	142	138
9	86	86

H,5,6

h	$10F_o$	$10F_c$
0 L	0	37
1	529	499
2 L	0	16
3	236	230
4	141	141
5	77	81
6	60	58
7	286	290
8	39	51

H,6,6

h	$10F_o$	$10F_c$
0	45	17
1	317	298
2	63	73
3	184	181
4	228	225
5	187	185
6	211	214
7	63	69
8	49	52

H,7,6

h	$10F_o$	$10F_c$
0	180	162
1	269	252
2	55	36
3	226	224
4	176	179
5	211	214
6	105	100
7	153	156

H,8,6

h	$10F_o$	$10F_c$
0	328	305
1	158	153
2	148	143
3	146	155
4	83	86
5	95	105
6	180	185
7	91	90

H,9,6

h	$10F_o$	$10F_c$
0	230	220
1	104	115
2	53	48
3	112	121
4	166	161
5	190	192
6	79	73

H,10,6

h	$10F_o$	$10F_c$
0	168	169
1	99	106
2	167	171
3	113	124
4 L	0	23
5	129	131

H,11,6

h	$10F_o$	$10F_c$
0 L	36	21
1	194	199
2	140	144
3	127	120

H,0,7

h	$10F_o$	$10F_c$
1	146	155
2	225	227
3	158	162
4	72	75
5	52	40
6	138	130
7	56	53
8	85	87

H,1,7

h	$10F_o$	$10F_c$
0	40	15
1	238	251
2	49	66
3	158	164
4	40	42
5	212	217
6	115	119
7 L	38	45
8	128	124

H,2,7

h	$10F_o$	$10F_c$
0	245	265
1 L	29	15
2	56	63
3	100	97
4	261	267
5	80	83
6	113	110
7	148	144
8	179	179

H,3,7

h	$10F_o$	$10F_c$
0	94	94
1	200	198
2	167	169
3	203	201
4	132	135
5	158	160
6	59	50
7	148	141
8	116	117

H,4,7

h	$10F_o$	$10F_c$
0	358	357
1	156	163
2	40	46
3	119	119
4	265	271
5	81	82
6	52	51
7	142	150

H,5,7

h	$10F_o$	$10F_c$
0	55	49
1	184	187
2 L	34	51
3	176	171
4	57	27
5	257	251
6	64	48
7	169	168

H,6,7

h	$10F_o$	$10F_c$
0 L	39	11
1	171	167
2	127	132
3	229	225
4	48	65
5	115	122
6	97	94
7	153	163

H,7,7

h	$10F_o$	$10F_c$
0 L	[illegible]	4
1	197	192
2	165	156
3	100	96
4	68	58
5	139	140
6	145	154

H,8,7

h	$10F_o$	$10F_c$
0	181	168
1	74	75
2	138	138
3	73	66
4	190	188
5	126	131

H,9,7

h	$10F_o$	$10F_c$
0	76	70
1	63	46
2	132	135
3	62	60
4	97	98

H,10,7

h	$10F_o$	$10F_c$
0	238	220
1	101	106
2	50	66

h		$10F_o$	$10F_c$
	H,0,8		
0		422	460
1		41	56
2		48	38
3		69	69
4		190	198
5		157	157
6		157	155
7	L	33	6
	H,1,8		
0		145	164
1		251	275
2		158	167
3		244	261
4	L	37	33
5		193	193
6		109	108
7		230	230
	H,2,8		
0	L	0	23
1		97	102
2		249	270
3	L	0	32
4		221	220
5		43	52
6		200	202
	H,3,8		
0		92	98
1		204	211
2		165	173
3	L	34	48
4		191	196
5		60	66
6		181	193
	H,4,8		
0		131	135
1		176	177
2		254	262
3	L	43	49
4		96	94
5		100	87
6		228	239
	H,5,8		
0		45	57
1		140	139
2		91	99
3		228	222
4		106	103
5		130	117
	H,6,8		
0		183	190
1		107	101
2		169	169
3		144	137
4	L	36	50
5		161	166
	H,7,8		
0		126	132
1		151	145
2		94	97
3		229	220
4		101	96
	H,8,8		
0		133	120
1	L	39	63
2		250	244
	H,0,14		
0	L	36	51

To compare vuagnatite and conichalcite, the transformations are :

$\underline{a}_v = \underline{a}_c$ $\quad x_v = x_c + 1/4$

$\underline{b}_v = \underline{c}_c$ $\quad y_v = z_c + 1/4$

$\underline{c}_v = -\underline{b}_c$ $\quad z_v = y_c - 1/4$