

>>> copy master bdf ludwig.000 --> ludwig.aal

*** Begin LISTFC ***

Input ludwig.aal with file history... LUDWIG

STARTX 19/ 9/92 19: 3:49 ADDATM 19/ 9/92 19: 4:14 ADDRFX 19/ 9/92 19: 4:37
CRYLSQ 19/ 9/92 19: 5:52 CRYLSQ 19/ 9/92 19: 9: 0 CRYLSQ 19/ 9/92 19:11:52
CRYLSQ 19/ 9/92 19:14:58 FC 19/ 9/92 21:55:28 FC 19/ 9/92 21:57:36
SORTRF 19/ 9/92 22:30:10 FOURR 6/ 8/93 15:39:38 CRYLSQ 6/ 8/93 16: 1:24
FOURR 6/ 8/93 16: 1:52

LISTFC CONTROL PARAMETERS

ITEMS TO BE LISTED 1 1701 1800 1305
OUTPUT FORMATS ARE I 5 I 5 I 5 I 5
ITEMS HAVE BEEN SCALED 1.00 10.00 10.00 10.00
CHARS/LINE LINES/PAGE 70 54
FREL AND SIGF SCALE(S) 1 .1220

IRWIN & PETERSON
FOR DEPOSIT

0,0,L			
1	943	939	0
2	224	1919	6
3	410	411	2
4	859	873	2
5	245	247	2

0,2,L			
0	276	267	0
1	378	373	1
2	159	166	1
3	211	216	2
4	81	81	1
5	106	102	1

0,4,L			
0	323	311	1
1	563	542	1
2	156	156	2
3	350	349	2
4	111	109	1
5	181	184	2

0,6,L			
0	68	61	0
1	31	28	1
2	29	23	2
3	33	14	3
4	18	11	8
5	17	1	11

0,8,L			
0	1103	1068	2
1	707	703	2
2	777	771	2
3	420	415	2
4	425	425	3
5	249	254	3

0,10,L			
0	277	270	2
1	74	66	0
2	221	222	2
3	62	59	1
4	127	123	1

0,12,L			
0	172	178	2
1	217	219	2
2	145	148	1
3	156	157	2
4	100	102	2

0,14,L			
0	230	245	2
1	423	419	2
2	184	185	2
3	296	294	3
4	106	98	2

0,16,L			
0	175	175	2
1	295	300	2
2	155	153	2
3	222	227	2

0,18,L			
0	302	305	3
1	179	179	2
2	265	268	3
3	157	157	2

0,20,L			
0	50	49	2
1	139	138	1
2	50	43	2

0,22,L			
0	78	73	2

1,1,L			
1	289	288	1
2	101	101	1
3	152	157	2
4	50	48	2
5	75	71	2

1,2,L			
1	92	115	0
2	474	481	1
3	154	152	2

4	235	237	2
5	92	90	2

1,3,L			
1	318	322	1
2	53	37	0
3	217	216	2
4	0	3	121
5	99	96	2

1,4,L			
1	117	112	1
2	187	182	2
3	81	79	1
4	97	97	1
5	50	48	2

1,5,L			
1	179	184	1
2	205	197	2
3	101	100	1
4	106	103	1
5	58	55	2

1,6,L			
1	543	541	2
1	551	541	1
1	554	541	1
2	498	489	2
3	297	295	2
4	261	261	2
5	173	171	2

1,7,L			
1	1002	960	2
2	183	181	2
3	507	504	2
4	82	80	1
5	263	254	3

1,8,L			
1	414	415	2
2	310	314	2
3	243	244	2
4	184	179	2

	1,8,L			1,16,L			1 362 348 1
							2 49 49 0
5	148 145	2	1	303 305	3		3 179 179 2
	1,9,L		2	144 145	1		4 27 25 2
			3	238 239	2		5 86 83 2
							2,3,L
1	48 51	1		1,17,L			1 318 302 1
2	209 208	2					2 56 56 0
3	35 32	2	1	63 61	2		3 121 126 1
4	113 111	1	2	12 6	12		4 29 28 2
			3	41 41	2		5 63 63 2
	1,10,L						2,4,L
1	246 240	2		1,18,L			0 1483 1392 1
2	147 143	2	1	103 98	1		1 571 557 1
3	162 160	2	2	112 107	1		2 980 976 2
4	96 93	2	3	82 80	2		3 325 319 2
							4 501 488 2
	1,11,L			1,19,L			5 205 202 2
1	377 379	2	1	124 123	1		2,5,L
2	39 38	2	2	58 57	2		1 223 216 1
3	231 230	2					2 477 485 2
4	43 39	2		1,20,L			3 90 91 1
							4 223 219 2
	1,12,L		1	351 357	3		5 48 45 2
1	497 503	2	2	269 271	3		2,6,L
2	311 308	2					0 554 547 1
3	347 348	3		1,21,L			1 451 441 2
4	205 206	2	1	207 208	2		2 372 377 2
							3 248 248 2
	1,13,L			2,0,L			4 195 191 2
1	146 141	1	0	148 151	0		5 141 138 2
2	198 201	2	1	1353 1275	5		2,7,L
3	105 100	1	2	61 52	0		1 107 107 1
4	127 126	2	3	624 636	2		2 42 41 1
			4	61 64	1		3 60 58 1
	1,14,L		5	315 314	3		4 28 23 3
1	216 213	2					5 35 33 3
2	160 157	2		2,1,L			2,8,L
3	160 158	2	1	139 131	1		0 164 160 2
4	113 110	2	2	27 22	1		
			3	48 43	1		
	1,15,L		4	17 12	5		
1	307 309	2	5	24 22	3		
2	76 74	1					
3	222 223	2		2,2,L			
4	59 56	2	0	86 92	0		

					4,14,L		5	24	16	6
	4,7,L									
				0	9	7	12		5,2,L	
2	98	100	1	1	147	147	1			
3	71	72	1	2	17	18	6	1	791	808
4	61	57	2	3	104	105	1	2	449	447
5	42	44	3	4	37	34	3	3	418	419
								4	243	245
	4,8,L				4,15,L			5	247	242
0	715	702	2	1	39	33	2		5,3,L	
1	388	388	2	2	50	51	2			
2	553	541	2	3	28	27	3	1	832	845
3	269	261	2					2	36	37
4	323	325	3		4,16,L			3	466	465
								4	44	39
	4,9,L			0	189	194	2	5	249	245
				1	286	291	3			
1	27	29	2	2	174	170	2		5,4,L	
2	106	107	1	3	222	222	2			
3	25	21	3					1	216	217
4	65	65	2		4,17,L			2	130	130
								3	125	128
	4,10,L			1	15	13	6	4	78	76
				2	14	0	12	5	77	74
0	812	817	2	3	19	10	8			
1	333	347	2						5,5,L	
2	631	631	2		4,18,L			1	244	251
3	229	228	2					2	393	392
4	381	376	3	0	525	537	3	3	153	159
				1	94	93	1	4	222	219
	4,11,L			2	469	464	3	5	99	96
1	128	131	1		4,19,L				5,6,L	
2	99	100	1							
3	93	91	1	1	80	78	2	1	294	292
4	69	68	2	2	102	102	2	2	252	246
								3	193	187
	4,12,L				4,20,L			4	153	150
0	150	149	2	0	25	21	3			
1	18	12	5	1	7	1	20		5,7,L	
2	127	128	1							
3	22	20	6		4,21,L			1	156	150
4	88	90	2					2	107	105
				1	49	47	2	3	83	82
	4,13,L							4	50	51
					5,1,L					
1	17	10	3						5,8,L	
2	44	45	2	1	102	107	1			
3	10	5	7	2	91	88	0	1	185	188
4	24	30	6	3	52	54	1			
				4	45	45	2			

								6,3,L			
5,8,L				5,16,L							
2	128	127	1	1	262	264	2	1	25	15	2
3	129	130	1	2	314	313	3	2	88	88	1
4	87	87	2	3	210	210	2	3	20	20	3
								5			
								18 15 9			
5,9,L				5,17,L				6,4,L			
1	59	55	1	1	144	144	1				
2	126	122	1	2	12	6	9	0	1226	1260	2
3	33	35	2	3	113	106	2	1	427	431	2
4	64	63	2					2	904	901	2
				5,18,L				3			
				1				78 79 2			
				2				61 60 2			
				5,19,L				1			
				1				57 56 2			
				2				86 87 2			
				5,20,L				6,5,L			
				1				94 98 2			
				6,0,L				1			
				0				151 146 1			
				1				406 404 2			
				2				79 86 0			
				3				265 265 2			
				4				19 4 8			
				5				145 149 2			
				6,1,L				1			
				1				91 95 0			
				2				67 67 1			
				3				51 52 1			
				4				49 34 2			
				5				35 34 3			
				6,2,L				2			
				0				50 21 0			
				1				240 239 2			
				2				12 17 8			
				3				138 139 1			
				4				19 12 8			
				5				76 69 2			
				5,12,L				6,6,L			
				0				273 278 2			
				1				228 230 2			
				2				211 214 2			
				3				150 151 2			
				4				128 124 1			
				6,7,L				2			
				1				116 115 1			
				2				137 136 1			
				3				81 78 1			
				4				88 84 2			
				6,8,L				1			
				0				85 84 1			
				1				277 282 2			
				2				82 78 1			
				3				190 188 2			
				4				65 69 2			
				6,9,L				2			
				1				121 116 1			
				2				130 133 1			
				3				77 73 2			
5,8,L				5,16,L				6,3,L			
2	128	127	1	1	262	264	2	1	25	15	2
3	129	130	1	2	314	313	3	2	88	88	1
4	87	87	2	3	210	210	2	3	20	20	3
								4			
								53 51 2			
								5			
								18 15 9			
5,9,L				5,17,L				6,4,L			
1	59	55	1	1	144	144	1				
2	126	122	1	2	12	6	9	0	1226	1260	2
3	33	35	2	3	113	106	2	1	427	431	2
4	64	63	2					2	904	901	2
				5,18,L				3			
				1				78 79 2			
				2				61 60 2			
				5,19,L				1			
				1				57 56 2			
				2				86 87 2			
				5,20,L				6,5,L			
				1				94 98 2			
				6,0,L				1			
				0				151 146 1			
				1				406 404 2			
				2				79 86 0			
				3				265 265 2			
				4				19 4 8			
				5				145 149 2			
				6,1,L				2			
				1				91 95 0			
				2				67 67 1			
				3				51 52 1			
				4				49 34 2			
				5				35 34 3			
				6,2,L				3			
				0				50 21 0			
				1				240 239 2			
				2				12 17 8			
				3				138 139 1			
				4				19 12 8			
				5				76 69 2			
				5,12,L				6,6,L			
				0				273 278 2			
				1				228 230 2			
				2				211 214 2			
				3				150 151 2			
				4				128 124 1			
				6,7,L				2			
				1				116 115 1			
				2				137 136 1			
				3				81 78 1			
				4				88 84 2			
				6,8,L				1			
				0				85 84 1			
				1				277 282 2			
				2				82 78 1			
				3				190 188 2			
				4				65 69 2			
				6,9,L				2			
				1				121 116 1			
				2				130 133 1			
				3				77 73 2			
5,8,L				5,16,L				6,3,L			
2	128	127	1	1	262	264	2	1	25	15	2
3	129	130	1	2	314	313	3	2	88	88	1
4	87	87	2	3	210	210	2	3	20	20	3
								4			
								53 51 2			
								5			
								18 15 9			
5,9,L				5,17,L				6,4,L			
1	59	55	1	1	144	144	1				
2	126	122	1	2	12	6	9	0	1226	1260	2
3	33	35	2	3	113	106	2	1	427	431	2
4	64	63	2					2	904	901	2
				5,18,L				3			
				1				78 79 2			
				2				61 60 2			
				5,19,L				1			
				1				57 56 2			
				2				86 87 2			
				5,20,L				6,5,L			
				1				94 98 2			
				6,0,L				1			
				0				151 146 1			
				1				406 404 2			
				2				79 86 0			
				3				265 265 2			
				4				19 4 8			
				5				145 149 2			
				6,1,L				2			
				1				91 95 0			
				2				67 67 1			
				3				51 52 1			
				4				49 34 2			
				5				35 34 3			
				6,2,L				3			
				0				50 21 0			
				1				240 239 2			
				2				12 17 8			
				3				138 139 1			
				4				19 12 8			
				5				76 69 2			
				5,12,L				6,6,L			
				0				273 278 2			
				1				228 230 2			
				2				211 214 2			
				3				150 151 2			
				4				128 124 1			
				6,7,L				2			
				1				116 115 1			
				2				137 136 1			
				3				81 78 1			
				4				88 84 2			
				6,8,L				1			
				0				85 84 1			
				1				277 282 2			
				2				82 78 1			
				3				190 188 2			
				4				65 69 2			
				6,9,L				2			
				1				121 116 1			
				2				130 133 1			
				3				77 73 2			

					6,17,L		4	37	35	3
	6,9,L							7,6,L		
				1	97	100	1			
4	87	85	2	2	64	67	2			
	6,10,L				6,18,L					
0	34	23	2	0	76	76	2	1	212	207
1	296	306	2	1	241	245	2	2	237	229
2	14	13	10	2	62	60	2	3	146	142
3	207	203	2					4	156	151
4	6	7	13		6,19,L					
	6,11,L			1	58	60	2	1	671	685
1	160	161	2	2	144	144	1	2	73	73
2	104	103	1		6,20,L			3	443	444
3	116	118	1					4	70	65
4	75	72	2	0	110	105	1		7,8,L	
	6,12,L			1	154	154	2	1	224	223
0	294	300	2					2	199	197
1	338	344	2		7,1,L			3	158	158
2	252	248	2	1	349	349	2	4	129	129
3	255	252	2	2	216	223	2		7,9,L	
4	178	176	2	3	222	228	2	1	206	203
	6,13,L			4	136	138	1	2	295	295
1	50	52	2					3	148	149
2	101	101	1		7,2,L			4	191	189
3	30	38	5	1	166	156	2		7,10,L	
	6,14,L			2	424	436	2	1	242	238
0	350	354	2	3	115	117	1	2	183	184
1	119	118	1	4	251	257	2	3	179	175
2	296	296	3					4	128	128
3	108	105	2	1	116	114	1		7,11,L	
	6,15,L			2	242	243	2	1	297	304
0	210	207	2	3	62	58	1	2	36	35
1	164	162	2	4	143	134	1	3	201	201
2	166	161	2					4	10	14
	6,16,L				7,4,L				7,12,L	
0	71	70	1	1	131	137	1	1	324	328
1	18	24	6	2	153	158	2	2	134	133
2	61	61	2	3	88	91	1	3	252	246
3	17	12	10	4	99	94	2		7,13,L	
					7,5,L			1	10	12
0	123	122	1						13	
1	43	43	2							
2	82	81	1							

				8,2,L			8,9,L				
7,13,L				0	129	135	1	1	15	1	4
2	55	53	2	1	230	221	2	2	138	134	1
3	7	12	21	2	102	103	1	3	19	2	7
				3	142	145	1	4	96	89	2
7,14,L				4	67	66	2				
				8,3,L			8,10,L				
1	158	162	2				0	266	265	2	
2	98	96	1				1	105	105	1	
3	127	127	1	1	116	114	1	2	220	220	2
				2	107	110	1	3	89	88	2
7,15,L				3	77	78	1	4	147	147	2
				4	67	70	2				
1	276	277	3				8,11,L				
2	120	118	1				1	129	130	1	
3	214	207	2	8,4,L			2	114	111	1	
				0	103	106	1	3	102	100	2
7,16,L				1	392	390	2				
				2	95	92	1	8,12,L			
1	355	355	3	3	258	260	2				
2	156	157	2	4	86	84	2				
3	287	287	3				0	77	76	1	
				8,5,L			1	114	114	1	
7,17,L							2	70	68	2	
1	128	130	1	1	185	197	2	3	94	93	2
2	41	35	2	2	12	14	8				
				3	128	128	1	8,13,L			
				4	15	8	12				
7,18,L							8,6,L				
1	74	74	2				1	65	64	1	
2	79	80	2	0	17	20	6	2	19	21	8
				1	60	61	1	3	54	51	2
7,19,L				2	17	14	7	8,14,L			
				3	41	36	2				
1	124	122	1	4	13	3	11	0	180	178	2
				8,7,L			8,15,L				
8,0,L											
0	1200	1219	2	1	162	161	2	1	189	188	2
1	255	263	2	2	122	117	1	2	173	172	2
2	924	945	2	3	116	114	1	3	152	150	2
3	191	193	2	4	83	81	2				
4	546	544	3				8,8,L				
8,1,L							8,16,L				
1	193	194	2	0	540	551	2				
2	167	171	2	1	374	375	2	0	126	123	1
3	118	117	1	2	446	443	2	1	205	209	2
4	103	103	1	3	276	270	3				
				4	302	291	3				

								9,14,L							
8,16,L				9,6,L											
2	108	112	2	1	287	294	2	1	123	123	1	2	113	113	1
				2	273	266	2	3	103	100	2				
8,17,L				3	217	210	2	9,15,L							
1	82	88	2	4	185	180	2								
2	63	65	2	9,7,L				1	121	124	1	2	28	27	3
8,18,L				1	359	368	2	9,16,L							
0	250	250	2	2	267	267	3								
1	140	140	1	3	243	234	2	1	129	132	1	2	114	113	2
8,19,L				4	170	170	2	9,17,L							
				9,8,L											
1	108	111	2	1	191	192	2								
				2	168	165	2	1	13	3	9				
9,1,L				3	142	141	1	9,18,L							
1	66	68	1	4	121	117	2								
2	8	12	13	9,9,L				1	62	56	2				
3	37	33	2					10,0,L							
4	0	14	121	1	118	117	1								
9,2,L				2	13	12	11	0	39	30	1				
				3	87	89	2	1	613	628	2				
1	216	209	2	4	15	18	6	2	19	10	4				
2	181	180	2	9,10,L				3	431	424	2				
3	150	151	2					4	24	19	3				
4	125	125	1	1	147	147	1	10,1,L							
				2	75	72	2								
9,3,L				3	113	115	2								
				9,11,L											
1	357	368	2					1	126	125	1				
2	148	151	1					2	147	145	1				
3	236	245	2	1	143	140	1	3	91	87	1				
4	112	112	2	2	15	3	10	4	97	97	2				
				3	96	96	2	10,2,L							
9,4,L				9,12,L											
1	44	39	1					0	36	37	2				
2	93	94	1	1	244	245	2	1	143	139	1				
3	37	30	2	2	233	231	2	2	32	30	2				
4	63	62	2	3	194	192	2	3	94	94	1				
9,5,L				9,13,L				10,3,L							
1	302	309	2	1	190	189	2	1	223	229	2				
2	284	289	2	2	233	230	2	2	99	101	1				
3	217	223	2	3	155	151	2								
4	189	189	2												

	11,11,L				12,4,L			1	9	8	19
								2	58	56	2
2	99	96	2	0	157	159	2		12,13,L		
3	87	87	2	1	188	192	2				
				2	129	125	1	1	27	21	3
	11,12,L			3	140	139	1	2	66	66	2
1	72	72	2		12,5,L				12,14,L		
2	173	168	2								
				1	209	204	2	0	71	67	2
	11,13,L			2	74	73	2	1	178	171	2
				3	163	158	2				
1	76	70	2						13,1,L		
2	70	71	2		12,6,L						
								1	105	105	1
	11,14,L			0	5	5	31	2	184	184	2
				1	79	75	1	3	92	89	2
1	93	91	1	2	11	7	6				
2	113	109	2	3	65	59	2		13,2,L		
	11,15,L				12,7,L			1	220	221	2
1	92	91	2	1	161	163	2	2	229	228	2
				2	155	154	2	3	177	174	2
	11,16,L			3	126	130	2				
									13,3,L		
1	37	28	2		12,8,L			1	375	365	3
								2	74	74	2
	12,0,L			0	283	279	3	3	286	285	3
				1	131	122	1				
0	391	390	2	2	248	240	3		13,4,L		
1	151	149	2	3	105	103	2				
2	321	326	2					1	34	36	2
3	133	130	1		12,9,L			2	35	32	2
								3	28	31	3
	12,1,L			1	16	11	10				
				2	120	112	2		13,5,L		
1	74	75	1	3	13	11	13				
2	11	8	9					1	173	173	2
3	58	59	2		12,10,L			2	259	254	3
								3	139	143	2
	12,2,L			0	310	303	3				
				1	132	130	1		13,6,L		
0	69	71	1	2	269	262	3				
1	199	198	2					1	132	128	1
2	63	62	2		12,11,L			2	189	183	2
3	147	147	1					3	106	105	2
				1	201	196	2				
	12,3,L			2	156	158	2		13,7,L		
1	120	121	1		12,12,L			1	21	26	8
2	158	158	2								
3	99	98	2	0	65	61	2				

16,4,L

1 183 173 2

0 32 31 3

16,6,L

LISTFC LUDWIG 6/ 8/93 Page 15 XTAL3.0 SEP90/UNIX

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THE CRYSTAL STRUCTURE OF LUDWIGITE

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ABSTRACT

We have refined the structure of ludwigite with a crystal taken from the Crestmore quarry, California; it is close to the end member in composition, ideally Mg_2FeBO_5 . The sample has a formula $\text{Mg}_{1.76}\text{Fe}_{1.22}\text{Al}_{0.02}\text{BO}_5$ and unit-cell dimensions a 9.2411(6), b 12.2948(9), c 3.0213(3) Å, V 343.27(5) Å³. The structure was refined in space group *Pbam*, to a final $R_w = 0.023$ for 948 observed unique reflections. The very low Al content allows the refinement of the distribution of magnesium and iron in the structure without assumptions as to the location of aluminum.

Keywords: ludwigite, vonsenite, pinakiolite group, crystal structure, Crestmore quarry, California.

SOMMAIRE

Nous avons affiné la structure de la ludwigite avec un cristal provenant de la carrière Crestmore, en Californie, et dont la composition est voisine de la composition idéale, Mg_2FeBO_5 . La formule est en fait $\text{Mg}_{1.76}\text{Fe}_{1.22}\text{Al}_{0.02}\text{BO}_5$, et les paramètres réticulaires sont: a 9.2411(6), b 12.2948(9), c 3.0213(3) Å, V 343.27(5) Å³. L'affinement, dans le groupe spatial *Pbam*, a mené à un résidu final R_w de 0.023 pour 948 réflexions uniques observées. La teneur très faible en Al permet un affinement de la distribution du magnésium et du fer dans la structure sans avoir à adresser la question de la distribution de l'aluminium.

(Traduit par la Rédaction)

Mots-clés: ludwigite, vonsenite, groupe de la pinakiolite, structure cristalline, carrière Crestmore, Californie.

INTRODUCTION

We present here the results of a refinement of the crystal structure of ludwigite; in the sample selected, from the Crestmore quarry, California, there is almost no aluminum substituting for Fe^{3+} . Ludwigite, with an ideal formula $\text{Mg}_2\text{Fe}^{3+}\text{BO}_5$, is an end-member of the ludwigite–vonsenite ($\text{Fe}^{2+}_2\text{Fe}^{3+}\text{BO}_5$) series. Manganese, aluminum and titanium commonly are found to substitute for magnesium and iron. This sample of ludwigite contains only magnesium and iron (with very minor aluminum), and the structure refinement provides information about the structure in the absence of the other substituents.

BACKGROUND INFORMATION

Takéuchi *et al.* (1950) solved the structure of ludwigite. It belongs to the pinakiolite group of minerals, in which metal ions are octahedrally coordinated by oxygen. The octahedra are linked together by edge-sharing to form what have been described as walls (*e.g.*, Bovin *et al.* 1981). Figure 1 shows the structure of

ludwigite viewed down the c axis. Swinnea & Steinfink (1983) refined the structure of synthetic vonsenite (Fe_3BO_5) and, on the basis of Mössbauer spectroscopy, concluded that ferrous and ferric iron occur in sites $M2$ and $M4$, whereas only ferrous iron occupies $M1$ and $M3$. They suggested that the distance between nearest-neighbor $M2$ and $M4$ sites of 2.79 Å is short enough for electron-hopping to occur. Norrestam *et al.* (1989) studied aluminian ludwigite and concluded, on the basis of site refinement of X-ray data and bond-valence calculations, that Mg occupies all four metal sites. They assumed that the aluminum is evenly distributed over all four sites. Bonazzi & Menchetti (1989) studied three structures in the ludwigite–vonsenite series and described the variation of cell dimensions and bond lengths with composition. Takéuchi & Kogure (1992) described the structure of a specimen of aluminian ludwigite and assigned aluminum to the $M4$ site.

EXPERIMENTAL

The crystal used is from the Crestmore quarry, Riverside, California, and was provided by the Canadian

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