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The crystal structure of paragonite-$2M_1$

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Abstract

The structure of a near end member paragonite-$2M_1$ was refined in $C2/c$ symmetry to a residual of 4.5% with 698 non-zero independent reflections. Attempted refinement in Cc symmetry was not successful. Tetrahedral Si,Al cations are disordered, and the mean T–O distances are in accord with prediction. The small interlayer Na cation facilitates a larger tetrahedral rotation angle (16.2°), smaller b-repeat (8.898Å), and smaller interlayer separation (3.053Å) than observed for muscovite-$2M_1$. It also allows an offset of adjacent 2:1 layers across the interlayer gap that significantly reduces the β angle and is due to mutual repulsion between oxygen anions brought into proximity by tetrahedral tilting.

Introduction

Paragonite, the Na analogue of muscovite, is an abundant rock-forming mineral in low-grade and medium-grade metamorphic rocks. There is a solid solution between paragonite and muscovite and a slightly asymmetric unmixing solvus. Naturally occurring end member paragonite has not been reported.

The most abundant polytype for paragonite is $2M_1$, although the 3T form also has been recognized in nature and the 1M form can be made synthetically. The $2M_1$ and 3T paragonite polytypes may coexist with very similar compositions (Nakamura and Kihara, 1977). Burnham and Radoslovich (1964) refined the structures of coexisting natural sodian muscovite-$2M_1$ ($K_{0.65}Na_{0.35}$) and potassian paragonite-$2M_1$($Na_{0.85}K_{0.15}$) by single crystal X-ray techniques. Soboleva *et al.* (1976) used high voltage texture electron diffraction patterns to refine the structure of a fine grained synthetic paragonite-1M ($Na_{0.91}K_{0.09}$). Sidorenko *et al.* (1977a,b) applied the same technique for the refinement of natural fine grained $2M_1$ ($Na_{0.06}K_{0.10}Ca_{0.03}\square_{0.27}$) and 3T ($Na_{0.71}K_{0.16}Ca_{0.03}\square_{0.10}$) forms of paragonite. This paper reports refinement of a near end member paragonite-$2M_1$ ($Na_{0.92}K_{0.04}Ca_{0.02}\square_{0.02}$) structure by single crystal X-ray methods. The research was investigated in order to provide more accurate parameters of a paragonite without appreciable interlayer K or vacancies to serve as a reference for comparison with the structures of other Na-micas. Attention will be focused on the interlayer region.

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Experimental

Several homogeneous paragonites of near end member composition (~4 mole% muscovite) were kindly furnished by Prof. Dr. Martin Frey of the University of Basel and Professor C. V. Guidotti of the University of Maine. A suitable but thin lath-shaped single crystal 0.32 × 0.25 × 0.018 mm in size was obtained from sample PVB 1705, originally collected by Prof. Dr. Peter Bearth of the University of Basel from a glaucophane-bearing metamorphosed eclogite from the ophiolite zone of Zermatt-Saas Fee in the Swiss Alps. The occurrence is described by Bearth (1973) and Bearth and Stern (1979). An electron microprobe analysis (Table 1) of this sample by C. A. Geiger of this department shows that only one mica is present and gives a resultant formula of $(Na_{0.916}K_{0.042}Ca_{0.018}\square_{0.024})(Al_{1.990}Fe_{0.028}Mg_{0.013}Ti_{0.003})_{2.034}(Si_{2.939}Al_{1.061})O_{10}(OH)_2$.

Cell dimensions of a = 5.128(2)Å, b = 8.898(3)Å, c = 19.287(9)Å, and β = 94.35(3)° were obtained by least squares refinement of 15 reflections on a Nicolet $P2_1$ automated single crystal diffractometer. These also indicate a near end member composition. Data for 5449 reflections were obtained out to 2θ = 60° in all eight octants of the limiting sphere. The $2\theta:\theta$ variable scan technique with monochromatic Mo$K\alpha$ radiation was used. Crystal and electronic stability were checked after every 50 reflections by monitoring a standard reflection. Integrated intensities were corrected for Lp and absorption effects and symmetry-averaged to 698 non-zero independent monoclinic reflections. The absorption correction was produced by the empirical ψ scan technique in which the data are compared to complete ψ scans (10° increments of ϕ) for selected reflections spaced at 2θ

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TABLE 2. Observed and calculated structure amplitudes

K	L	10FO	10FC
	H = 0		
0	2	545	613
0	4	683	721
0	12	517	534
0	14	812	866
0	16	755	778
0	18	190	196
0	20	696	670
2	0	328	317
2	1	635	567
2	2	676	611
2	3	672	661
2	4	1025	1035
2	5	1223	1225
2	6	115	125
2	7	342	363
2	9	258	275
2	10	382	416
2	11	134	149
2	12	195	212
2	13	420	450
2	15	392	413
2	16	358	380
2	18	250	251
2	23	221	197
4	1	309	290
4	2	465	421
4	3	502	445
4	4	849	811
4	5	241	241
4	6	462	454
4	7	308	323
4	9	237	258
4	10	790	814
4	11	179	204
4	12	730	769
4	13	611	621
4	14	463	488
4	15	305	319
4	16	224	227
4	17	287	288
4	18	282	269
4	19	213	216
4	20	182	151
4	23	277	246
4	24	295	272
6	0	2741	2729
6	1	552	495
6	2	529	497
6	3	260	233
6	4	239	218
6	5	364	372
6	6	940	936
6	8	677	678
6	9	456	479
6	10	769	779
6	11	284	291
6	13	244	246
6	14	815	832
6	15	191	231
6	16	553	556
6	22	643	566
8	0	372	360
8	1	187	184
8	2	404	398
8	3	293	270
8	4	275	257
8	5	527	524
8	6	147	141
8	9	294	290
8	13	285	295
8	15	297	292
8	18	216	197
8	20	220	202
10	2	230	224
10	4	418	410
10	6	311	298
10	7	211	216
10	13	243	221
10	14	322	330
12	0	668	673
12	1	291	307
12	2	278	259
12	3	182	169
12	5	270	304
12	6	333	336
12	8	434	485
	H = 1		
1	0	790	759
1	1	472	458
1	-1	1144	1149
1	2	249	227
1	-2	336	322
1	-3	661	693
1	4	1159	1142
1	-4	855	891
1	5	1121	1105
1	-5	225	227
1	6	556	557
1	-6	1033	1015
1	-7	429	442
1	8	127	119
1	-8	219	230
1	-9	198	208
1	10	167	187
1	-10	237	242
1	11	270	287
1	-11	175	183
1	12	262	297
1	13	316	357
1	-13	122	161
1	14	439	477
1	-14	383	434
1	15	163	181
1	-15	510	553
1	17	229	220
1	-17	355	373
1	18	173	178
1	21	335	301
1	-21	163	156
1	-22	171	168
1	-23	389	322
1	24	186	152
1	-24	211	189
3	0	408	337
3	-4	229	201
3	5	1521	1523
3	-5	1091	1158
3	7	723	744
3	-7	732	739
3	-8	238	265
3	-9	1015	1054
3	10	157	186
3	-10	242	275
3	11	647	691
3	-11	2068	2154
3	13	736	755
3	-14	255	289
3	-15	250	237
3	17	876	896
3	-17	210	206
3	-18	194	190
3	19	347	334
3	-19	851	860
3	-21	272	229
3	-23	256	240
3	25	450	360
3	-25	268	225
5	0	474	464
5	1	384	355
5	-1	346	316
5	2	194	194
5	3	574	587
5	-3	216	197
5	4	538	534
5	-4	1015	955
5	5	610	635
5	-5	318	296

K	L	10FO	10FC	K	L	10FO	10FC	K	L	10FO	10FC
5	6	488	487	9	8	331	349	2	11	560	567
5	-6	771	737	9	-8	220	230	2	-11	153	153
5	7	403	392	9	10	294	308	2	-12	358	388
5	-7	135	132	9	-10	319	342	2	13	770	765
5	-8	163	177	9	11	310	322	2	-13	513	528
5	9	298	299	9	-11	742	772	2	14	235	250
5	-9	261	284	9	13	362	370	2	-14	437	455
5	-10	400	404	9	-13	654	698	2	-15	679	698
5	-11	162	176	9	14	258	250	2	16	286	295
5	12	172	190	9	-18	257	260	2	17	415	417
5	-13	311	338	9	-19	518	463	2	19	193	171
5	14	178	190	11	0	198	214	2	-19	254	251
5	-14	475	513	11	1	226	245	2	-25	242	186
5	-15	436	457	11	-2	221	242	4	0	754	729
5	16	143	136	11	3	219	251	4	1	340	334
5	-16	219	252	11	4	333	397	4	-1	433	400
5	-17	189	206	11	6	201	199	4	2	704	700
5	-18	147	162	11	-6	246	253	4	3	423	423
5	21	233	221	11	7	226	237	4	-3	375	343
5	22	262	240	11	8	205	188	4	4	162	178
5	-24	224	193	11	-13	207	267	4	-4	540	522
7	0	350	316					4	5	480	466
7	1	300	268					4	-5	1015	949
7	-1	1246	1198		H = 2			4	6	601	608
7	2	332	305					4	-6	808	779
7	-2	476	459	0	0	719	632	4	-7	427	410
7	3	817	787	0	8	1021	1074	4	8	360	351
7	-3	460	421	0	-8	777	820	4	-9	361	375
7	4	795	774	0	10	1577	1665	4	10	313	306
7	5	659	635	0	-10	1690	1761	4	-11	455	456
7	6	251	226	0	12	1900	1972	4	12	330	329
7	-6	372	379	0	-12	334	378	4	-12	521	553
7	-7	687	696	0	-14	703	719	4	13	370	380
7	8	383	370	0	-16	171	161	4	-14	560	593
7	-8	152	169	0	18	871	861	4	-15	498	518
7	10	321	335	0	-18	839	862	4	16	380	368
7	11	379	364	0	-20	467	462	4	17	164	198
7	13	672	683	0	-26	258	215	4	-17	179	172
7	-13	275	279	2	0	407	407	4	-18	172	169
7	14	356	368	2	1	396	430	6	0	624	612
7	-15	159	155	2	-1	403	382	6	1	137	114
7	17	233	227	2	2	317	322	6	-1	527	516
7	-17	321	309	2	3	463	488	6	2	440	407
9	0	452	450	2	-3	552	577	6	-2	1560	1608
9	1	675	619	2	4	302	310	6	3	350	347
9	-1	490	469	2	-5	572	634	6	-3	248	206
9	-2	230	232	2	6	229	244	6	4	1130	1062
9	3	1017	1002	2	-6	538	568	6	-4	969	937
9	-3	201	205	2	7	516	516	6	5	158	118
9	4	407	392	2	8	665	706	6	-5	194	192
9	-4	265	250	2	-8	612	594	6	6	455	402
9	-5	758	737	2	-9	480	469	6	-6	179	180
9	-6	190	188	2	10	750	776	6	7	205	218
9	-7	259	249	2	-10	520	525	6	8	575	566

K	L	10FO	10FC	K	L	10FO	10FC	K	L	10FO	10FC
6	-8	600	628	H = 3				3	-17	323	318
6	9	258	259					3	19	495	491
6	10	1099	1105	1	1	361	339	3	21	662	646
6	-10	1229	1271	1	-1	202	184	3	-23	430	395
6	-11	187	220	1	2	887	860	5	-1	476	450
6	12	1105	1118	1	-2	396	396	5	2	925	883
6	13	234	233	1	3	665	647	5	-2	625	599
6	-14	347	343	1	-3	917	871	5	3	302	277
6	-16	300	307	1	4	864	846	5	-3	962	935
6	17	241	242	1	-5	834	817	5	4	916	876
6	18	562	565	1	-6	417	403	5	-4	281	256
6	-18	548	552	1	7	306	300	5	5	177	147
6	-19	175	169	1	8	455	465	5	-5	530	504
6	-20	225	222	1	-8	213	214	5	-6	410	407
6	22	262	218	1	9	480	457	5	7	239	252
8	3	212	220	1	-9	465	484	5	-7	225	239
8	-4	166	170	1	10	190	177	5	8	629	640
8	-5	417	407	1	11	671	667	5	-8	368	356
8	6	189	182	1	-11	284	283	5	9	178	165
8	-6	304	293	1	12	370	390	5	-9	285	305
8	7	287	268	1	14	355	354	5	10	227	215
8	8	430	419	1	-14	456	452	5	11	315	305
8	-8	403	425	1	15	316	296	5	12	354	350
8	-9	238	254	1	-15	196	204	5	13	306	285
8	10	382	354	1	-16	230	223	5	14	395	411
8	-10	303	313	1	17	329	325	5	-14	202	204
8	11	318	326	1	-17	259	242	5	15	335	340
8	12	187	207	1	-18	229	233	5	17	238	236
8	-12	337	317	1	-20	206	195	5	-23	207	182
8	13	356	341	1	-23	187	141	7	1	173	210
8	-13	196	183	1	-24	327	292	7	-1	180	193
8	-14	200	200	1	-25	253	216	7	3	452	462
8	17	296	294	3	0	264	213	7	4	217	225
10	0	717	743	3	1	985	970	7	-4	236	240
10	1	247	226	3	-1	2756	2694	7	5	234	229
10	-1	211	195	3	2	179	148	7	-5	552	580
10	2	510	524	3	-2	389	295	7	-6	264	269
10	-4	411	409	3	3	362	364	7	9	462	430
10	5	230	225	3	5	665	650	7	-9	211	200
10	-5	364	353	3	-6	227	236	7	-10	235	259
10	6	334	366	3	7	1109	1058	7	-11	608	600
10	-6	435	452	3	-7	1096	1142	7	12	218	205
10	8	242	254	3	8	231	212	7	-13	285	283
10	-10	363	375	3	9	737	722	7	-14	305	311
10	12	334	317	3	-9	471	455	7	-15	330	339
10	-12	369	415	3	-10	223	220	7	-16	268	226
10	-14	480	504	3	11	165	202	7	17	248	215
12	-1	422	461	3	-11	908	930	7	-17	189	177
12	-2	737	787	3	12	223	213	9	0	316	277
12	3	333	350	3	-12	231	245	9	1	359	349
12	-4	456	488	3	13	856	888	9	-1	1052	1027
12	-5	335	341	3	-13	474	456	9	-2	391	362
				3	15	721	703	9	-3	217	213
				3	-15	814	826	9	4	213	196

K	L	10FO	10FC
9	5	410	403
9	-5	303	308
9	-6	395	384
9	7	545	594
9	-7	580	565
9	8	233	263
9	-9	569	575
9	-10	386	393
9	-11	437	435
9	12	307	313
9	-12	312	315
9	-13	301	274
9	-15	745	705
9	-16	235	248
11	-1	297	277
11	-3	335	345
11	4	225	209

H = 4

K	L	10FO	10FC
0	0	1046	1084
0	2	1500	1456
0	-2	1085	1106
0	4	325	311
0	-4	347	326
0	6	247	227
0	-6	1130	1098
0	8	1408	1409
0	10	443	441
0	-10	328	355
0	12	391	386
0	-12	1468	1490
0	-14	692	695
0	-18	272	274
0	-20	701	652
2	0	540	510
2	-1	703	662
2	2	498	488
2	-2	637	592
2	3	575	562
2	-3	243	240
2	4	708	690
2	5	459	436
2	-5	762	741
2	6	255	260
2	-6	524	507
2	-7	915	904
2	-8	200	175
2	-9	156	156
2	-11	395	420
2	-13	245	256
2	-14	387	377
2	15	213	200
2	-15	234	248
2	-16	604	581
2	-17	261	266
2	21	270	218
4	0	481	473
4	-1	293	267
4	-2	677	638
4	3	445	446
4	-3	183	144
4	4	427	417
4	-4	270	250
4	-5	305	295
4	6	312	312
4	-6	198	208
4	7	207	199
4	-7	402	407
4	-8	380	370
4	-10	155	172
4	11	253	243
4	12	407	391
4	13	275	267
4	-15	219	233
4	-16	492	498
4	17	204	206
4	20	282	248
4	-22	246	205
6	0	481	438
6	1	187	150
6	-1	262	261
6	2	1150	1103
6	-2	568	561
6	3	305	279
6	-3	208	179
6	4	263	230
6	-4	436	428
6	-6	756	725
6	7	311	316
6	8	1208	1132
6	10	544	513
6	-11	330	312
6	12	357	356
6	-12	904	881
6	13	216	204
6	-14	606	578
6	-15	271	293
6	-20	539	542
8	0	446	436
8	-1	326	311
8	2	426	448
8	-2	274	250
8	3	277	297
8	-3	213	209
8	4	304	316
8	5	213	222
8	-5	400	400
8	6	250	258
8	-7	479	475
8	10	187	175
8	-11	263	259
8	-14	430	388
8	-16	273	260
10	2	297	297
10	-2	517	513
10	-8	360	355

H =

K	L	10FO	10FC
1	1	361	357
1	-1	177	177
1	2	352	386
1	6	337	324
1	-6	366	392
1	7	496	507
1	-7	402	393
1	-8	195	175
1	9	515	515
1	-9	256	248
1	10	250	235
1	-10	234	237
1	-11	279	305
1	12	448	428
1	-12	256	237
1	-13	287	297
1	-14	220	195
1	-15	315	326
1	16	292	271
1	-16	400	400
3	-1	306	315
3	-2	188	153
3	3	658	657
3	-3	1120	1089
3	-4	189	95
3	5	660	624
3	-5	612	611
3	7	218	214
3	9	382	409
3	-9	474	496
3	11	969	957
3	-11	1174	1112
3	13	256	285
3	15	238	232
3	17	439	445
3	-17	494	486
3	-19	305	283
5	-1	339	337
5	3	223	219
5	6	306	301

K	L	10FO	10FC
5	-6	315	321
5	7	492	457
5	-7	336	321
5	9	553	586
5	-9	385	382
5	10	356	352
5	-10	300	295
5	-11	386	388
5	12	285	310
5	-13	369	377
5	-14	235	227
5	-16	489	440
7	1	547	588
7	2	334	352
7	-2	235	225
7	4	211	203
7	7	385	420
7	-7	337	364
7	8	207	218
7	-13	253	254
9	2	278	317
9	-2	330	330
9	-3	848	908
9	-4	253	222
9	-5	280	296

H = 6

K	L	10FO	10FC
0	0	810	816
0	2	310	322
0	-2	857	863
0	6	948	1010
0	-6	302	307
0	-8	654	654
0	10	314	326
0	-10	351	382
0	12	747	727
0	-12	341	346
0	-16	523	515
2	1	468	461
2	-2	365	363
2	3	348	364
2	-3	278	283
2	-4	669	672
2	6	260	255
2	-6	276	298
2	7	310	323
2	-7	213	217
2	10	315	344
2	-10	252	261
2	11	271	254
2	13	228	183
4	2	326	330
4	3	333	337
4	-3	238	253
4	-4	442	482
4	-6	289	324
4	-7	313	337
4	10	315	322
4	-10	264	281
6	0	510	498
6	-2	666	689
6	-3	249	217
6	6	685	695
6	-8	541	567
6	-10	321	348

H = 7

K	L	10FO	10FC
1	-1	327	350
1	2	259	256
1	3	251	219
1	5	314	330
1	-8	282	269
3	1	819	905
3	-1	291	324
3	-3	393	391
3	-5	559	602

TABLE 4. Orientation of thermal ellipsoids for paragonite-$2M_1$

Atom	Axis	rms displacement	Angles with respect to X	Y	Z
T(1)	R1	0.078(4)Å	136(20)°	134(20)°	88(2)°
	R2	0.087(4)	134(20)	44(6)	91(3)
	R3	0.148(3)	87(2)	92(3)	178(2)
T(2)	R1	0.081(4)	82(35)	172(35)	89(3)
	R2	0.087(4)	8(33)	82(35)	91(2)
	R3	0.149(3)	87(2)	91(3)	179(3)
Al	R1	0.071(5)	125(11)	145(11)	89(3)
	R2	0.087(4)	144(10)	56(11)	96(3)
	R3	0.148(3)	81(2)	95(3)	174(3)
Na	R1	0.130(37)	44(23)	62(16)	124(16)
	R2	0.198(49)	47(26)	128(34)	71(20)
	R3	0.226(46)	98(27)	129(21)	139(13)
O(1)	R1	0.075(12)	37(20)	126(20)	88(4)
	R2	0.096(9)	54(20)	36(20)	88(6)
	R3	0.166(7)	83(4)	90(5)	177(4)
O(2)	R1	0.078(10)	97(21)	173(20)	87(5)
	R2	0.100(8)	7(20)	97(21)	91(6)
	R3	0.158(7)	87(6)	92(5)	177(5)
OH	R1	0.082(11)	140(26)	129(24)	96(9)
	R2	0.099(9)	130(26)	44(24)	73(6)
	R3	0.160(7)	92(5)	74(6)	162(6)
O(3)	R1	0.102(9)	104(11)	166(11)	84(6)
	R2	0.136(7)	14(11)	103(11)	92(10)
	R3	0.168(7)	89(10)	95(6)	174(6)
O(4)	R1	0.104(9)	96(16)	164(7)	75(5)
	R2	0.128(8)	6(16)	95(15)	93(9)
	R3	0.170(8)	90(8)	105(5)	165(6)
O(5)	R1	0.098(9)	66(15)	156(15)	93(5)
	R2	0.123(8)	25(14)	66(15)	99(7)
	R3	0.175(7)	95(6)	91(5)	171(6)