The Crystal Structures of Talc and Pyrophyllite.

By

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(With 2 figures.)

Introduction.

In 1930, in a preliminary paper Pauling[1]) suggested certain structural units for talc and pyrophyllite. No detailed paper, however, proving these structures has been published so far. The writer in connection with work on the vermiculite group recently investigated the two minerals completely. Since neither talc nor pyrophyllite are ever found with recognizable crystal faces, warped basal pinacoids excepted, only the powder method was available. A talc of light green color with large folia from Harford County, Maryland and a massive yellowish white variety from Vorwald, Styria were used. They gave practically identical diagrams. Two radiated yellowish pyrophyllites from Graves Mountain, Georgia, and Tres Cerritos, Mariposa County, California, respectively gave also identical (within the limit of error) diagrams. The analysis of the Tres Cerritos pyrophyllite, $Al_2Si_4O_{10}(OH)_2$, is given by Doelter[2]) as follows.

Al_2O_3	28.25
Fe_2O_3	0.18
SiO_2	65.96
TiO_2	trace
H_2O	5.27
H_2O at 105°	0.14
	99.80

Though no analyses are available for the talcs, the Harford talc, at least, cannot be very different from the theoretical formula $Mg_3Si_4O_{10}(OH)_2$. It was noticed that the minerals when ground in an agate mortar would give very unsatisfactory diagrams probably due to

1) Linus Pauling, The structure of the micas and related minerals. Proc. Nat. Acad. Sci. 16, 123. 1930.

2) Handbuch der Mineralchemie. 2, Teil 2, 121. 1917.

slipping and distortion of the layers. If filed with a fine file very good films were obtained. The samples mounted on silk thread were 0.6 to 0.7 mm. in diameter. A circular camera of 57.3 mm. radius was employed. The primary beam was effectively screened out so that spacings of 16 Å (FeK_α radiation) could have been recorded. A gas tube with *Cu* or *Fe* radiation was used, but *Fe* radiation was necessary to resolve some of the closely spaced lines. Exposure times with *Fe* radiation were about 24 hours at 35 KV and 6 MA.

X-ray data and their Interpretation.

The striking similarity of talc and pyrophyllite is revealed in tables I and II of their powder diagrams. Therefore, the following discussion of talc also applies equally well to pyrophyllite. The basal planes give sharp reflections which on account of their preferential orientation on the thread are 3 to 4 times as strong as the calculated ones in table III. This feature has already been discussed by the writer[1]) in the structure of dickite where other details of structure analyses of this type may be found.

If talc is built of layers as those suggested by Pauling, there will be vertical planes of symmetry in each layer (conventional monoclinic orientation). Such a layer being made up of a network of hexagons of Si_4O_{10} is base-centered monoclinic and belongs into space group C_{2h}^3 if the layers are stacked in such a way that the planes of symmetry are vertically above one another. Since the β angles of talc and pyrophyllite were unknown, different shifts of the layers in the + and — direction of the a axis had to be tried. It was thought at first that this shift might be twice the distance of those of muscovite[2]) and dickite[3]). This value, however, agreed only approximately with the powder diagrams. The exact values were found to be slightly smaller. Expressing the shift in degrees of a_0 it is 112° instead of 60° as in muscovite and dickite. This makes $\beta = 100°00' \pm 5'$ for talc and $99°55' \pm 5'$ for pyrophyllite.

The layers can also be stacked in such a fashion, that the individual planes of symmetry intersect at angles of 120° as shown in Fig. 1. A glide plane of symmetry bisects this angle. The resulting space group is C_{2h}^6, and the unit cell becomes twice as high (18.81 Å). All the reflections of $20\,l$, $13\,l$, $33\,l$ and $06\,l$ (l = even) remain the same as of corresponding

1) Z. Krist. **83**, 395. 1932, and Z. Krist. **83**, 78. 1932.
2) W. W. Jackson and J. West, Z. Krist. **76**, 221. 1931.
3) J. W. Gruner, Z. Krist. **83**, 397. 1932.

planes in C^3_{2h}. Those with l = odd are absent. Striking differences occur in the 11 l (l = odd or even) and in other planes which make space group C^6_{2h} highly probable. Theoretical and observed intensities for C^6_{2h} are recorded in table III for all planes with a spacing greater than 3.33 Å.

Table I. Powder diagram of talc from Harford County, Md.

$FeK_\alpha = 1.9321$. Radius of camera 57.3 mm.

No.	Θ	d	I	Indices
1	6° 12′	8.94 Å	5	002
2	11 02	5.05	1	020β, 004β
3	12 12	4.57	3	020, 004, 11$\bar{1}$
3a	14 40	3.82	1 very indistinct and broad	6 planes
4	16 39	3.37	3	006β, 113
5	18 24	3.060	10	006
6	20 57	2.702	1	20$\bar{4}\beta$, 132β
7	22 10	2.560	1 broad	13$\bar{2}$, 200, 008β
8	23 14	2.449	5	20$\bar{4}$, 132
9	24 42	2.312	1	008
10	26 12	2.188	2 broad	20$\bar{6}$, 134
11	27 40	2.081	1 broad	13$\bar{6}$, 204
12	28 17	2.039	1	0010β
13	30 12	1.920	0.5	136
14	31 29	1.850	3	0010
15	34 36	1.701	1 broad	0012β
16	35 30	1.664	3 broad	138
17	35 47	1.652	1—2	20$\overline{10}$
18	36 17	1.632	1 broad	several
19	38 44	1.544	2	0012
20	39 36	1.515	4	33$\bar{2}$, 060
21	40 08	1.499	1	33$\bar{4}$, 062, 330
22	41 23	1.461	1	1310
23	41 54	1.446	0.5	20$\overline{12}$
24	43 27	1.405	2	2010
25	44 38	1.375	3—4 broad	1312
26	46 44	1.327	1—2	0014
27	47 23	1.313	1	40$\bar{4}$, 260
28	48 32	1.289	2 broad	26$\bar{4}$, 400
29	49 54	1.263	0.5	33$\overline{10}$, 068, 20$\overline{14}$
30	51 45	1.230	1	13$\overline{14}$, 264, 2012
31	55 01	1.179	0.5	
32	56 01	1.165	0.5	0016
33	60 19	1.112	0.5	

Table II. Powder diagram of pyrophyllite from Tres Cerritos, Mariposa County, Calif.

$FeK_{\alpha} = 1.9321$. Radius of camera 57.3 mm.

No.	Θ	d	I	Indices
1	6° 11′	8.97 Å	3	002
2	11 12	4.97	0.5	020β, 004β
3	12 18	4.53	4	020, 004
4	13 33	4.12	2 very broad and	111, 11$\bar{2}$, 021, 11$\bar{1}$
5	14 31	3.85	0.5 indistinct	11$\bar{3}$, 022
6	16 48	3.34	2—3	006β, 113
7	18 33	3.037	8	006
8	20 29	2.761	0.5	13$\bar{2}\beta$, 200β
9	21 20	2.655	1	20$\bar{4}\beta$, 132β
10	22 30	2.524	2 broad	13$\bar{2}$, 200
11	23 44	2.400	3 broad	20$\bar{4}$, 132
12	24 59	2.287	2	008
13	26 48	2.142	1—2 broad	20$\bar{6}$, 134
14	27 48	2.071	1	204
15	28 12	2.044	1	13$\bar{6}$
16	28 41	2.013	0.5	0010β
17	30 54	1.881	0.5	136
18	31 54	1.828	3	0010
19	32 26	1.801	0.5	138β
20	35 05	1.681	0.5—1	0012β, incomplete
21	36 11	1.636	2—3	138
22	36 35	1.621	1—2	20$\overline{10}$
23	38 03	1.567	0.25 broad	208 incomplete
24	39 23	1.522	1	0012, 2010β
25	39 59	1.503	0.5	13$\overline{12}\beta$
26	40 35	1.485	2—3	060, 33$\bar{2}$
27	41 20	1.463	0.5—1	33$\bar{4}$, 062, 330
28	42 26	1.432	0.5	1310
29	42 53	1.419	0.5	20$\overline{12}$
30	44 32	1.377	3	2010
31	45 11	1.362	3	13$\overline{12}$
32	45 56	1.344	0.5	334
33	46 39	1.328	0.5	33$\bar{8}$, 066
34	47 39	1.307	1—2	0014
35	48 51	1.283	1	40$\bar{4}$, 260, 26$\bar{2}$
36	49 51	1.264	1—2	1312, 26$\bar{4}$, 400
37	50 24	1.254	0.5—1	20$\overline{14}$, 262
38	51 23	1.236	1	33$\overline{10}$, incomplete
39	53 12	1.206	0.5—1	13$\overline{14}$, 264
40	57 46	1.142	0.5	0016

Table III.

Theoretical and observed intensities for two molecules of talc and pyrophyllite. In comparing results allowance should be made for the glancing angle.

	Talc			Pyrophyllite		
Indices		Theoretical	Observed		Theoretical	Observed
	d	I	I	d	I	I
002	9.260	31	5	9.137	13	3
004	4.630	9		4.569	24	4
020	4.550	55	3	4.450	88	
$11\bar{1}$	4.531	35		4.432	33	
110	4.498	1		4.401	4	
021	4.418	57		4.324	53	2
$11\bar{2}$	4.310	24		4.219	58	
111	4.227	14	1	4.140	13	
022	4.084	5		4.001	22	0.5—1
$11\bar{3}$	3.929	68		3.851	64	
112	3.825	17		3.752	2	
023	3.663	2		3.593	1	
$11\bar{4}$	3.501	5		3.437	0	
113	3.399	65		3.338	60	2—3
006	3.086	202	10	3.046	156	8
130	2.617	16		2.560	3	
$20\bar{2}$	2.613	9		2.555	2	
200	2.588	44	1	2.532	70	2
$13\bar{2}$	2.578	89		2.522	141	
132	2.462	401	5	2.411	312	3
$20\bar{4}$	2.447	200		2.396	156	
202	2.387	5		2.338	15	
$13\bar{4}$	2.369	10		2.321	29	
008	2.315	27	1	2.284	48	2
134	2.197	218	2	2.154	174	1—2
$20\bar{6}$	2.178	119		2.136	87	
222	2.114	13		2.070	37	1
204	2.108	46	1	2.068	28	
$13\bar{6}$	2.089	90		2.049	56	1
136	1.915	43	0.5	1.880	20	0.5
$20\bar{8}$	1.897	21		1.863	10	
0010	1.852	44	3	1.829	65	3
206	1.833	3		1.800	0	
$13\bar{8}$	1.815	5		1.783	0	
138	1.663	298	3	1.635	235	3
$20\overline{10}$	1.647	150	1—2	1.619	118	1
208	1.593	10		1.567	4	0.25
$13\overline{10}$	1.579	21		1.553	8	
0012	1.544	35	2	1.523	22	1

Table III (continuation).

Indices	Talc			Pyrophyllite		
		Theoretical	Observed		Theoretical	Observed
	d	I	I	d	I	I
060	1.517	205	4	1.484	167	2—3
$33\bar{2}$	1.517	400		1.483	334	
330	1.499	113		1.467	79	
062	1.497	110	1	1.464	76	0.5—1
$33\bar{4}$	1.494	109		1.462	78	
1310	1.453	94	1	1.429	65	0.5
$20\bar{1}\bar{2}$	1.440	45	0.5	1.417	31	0.5
2010	1.396	224	2	1.374	192	3
$13\bar{1}\bar{2}$	1.384	449	3—4	1.362	386	3
334	1.367	30		1.340	16	0.5
066	1.361	30		1.334	16	0.5
$33\bar{8}$	1.355	31		1.328	17	
0014	1.323	50	1—2	1.305	42	1—2
$26\bar{2}$	1.311	40		1.283	25	
260	1.309	186	1	1.280	230	1
$40\bar{4}$	1.307	79		1.278	99	
400	1.294	213	2	1.266	184	
$26\bar{4}$	1.289	370		1.261	316	1—2
1312	1.281	80		1.261	108	
262	1.280	65		1.253	45	0.5—1
$20\bar{1}\bar{4}$	1.271	40		1.251	54	
068	1.269	45	0.5	1.244	28	1
$33\bar{1}\bar{0}$	1.262	35		1.238	26	
2012	1.234	55		1.216	42	
264	1.231	78	1	1.206	56	0.5—1
$13\bar{1}\bar{4}$	1.225	108		1.206	94	
0016	1.160	40	0.5	1.142	29	0.5

Below this spacing only those considered important are listed though others were calculated[1]).

It will be observed that probably due to preferred orientation the $20l$ planes often reflect with almost the same intensity as corresponding $13l$ planes. Also, the $11l$ planes are relatively very weak. This peculiarity is observed in all powder diagrams of layer silicates, whether

1) The intensities were computed with the structure factor formula $I' \infty j(F')^2 \infty j(A^2 + B^2)$ of R. W. G. Wyckoff. The F values were taken from Pauling's and Sherman's table of scattering factors for ions (Z. Krist. **81**, 27. 1932). $j = 1$ for $00l$, $h00$, $0k0$, $h0l$, and $j = 2$ for all other planes. The I' values were arbitrarily divided by 100. The I' values were calculated for shifts of 120° and are, therefore, slightly different from those for shifts of 112° parallel the a axis.

of micas, chlorites, kaolinites, or vermiculites. If C_{2h}^3 were the correct space group talc should show a distinct reflection at $d = 4.31$ Å for $11\bar{1}$ with $I' = 100$, and pyrophyllite at $d = 3.75$ Å for 111 with $I' = 122$ and at $d = 3.437$ for 112 with $I' = 78$. Even with $11\,l$ planes very weakly reflecting these lines should not be absent in the films.

Table IV. Atomic coordinates for C_{2h}^6. Four equivalent atomas for each position.

Atom	x	y	z
Mg_1	0°	0°	0°
Mg_2 or Al_1	0	120	0
Mg_3 or Al_2	0	—120	0
O_1	73	180	21
O_2	73	60	21
OH_1	73	—60	21
O_3	9	30	63.5
O_4	—171	30	63.5
O_5	99	120	63.5
O_6	—9	30	116.5
O_7	171	30	116.5
O_8	—99	120	116.5
O_9	—73	180	159
O_{10}	—73	60	159
OH_2	—73	—60	159
Si_1	—86	0	51.5
Si_2	94	60	51.5
Si_3	86	0	128.5
Si_4	—94	60	128.5

The atomic positions for C_{2h}^6 are given in table IV. The origin is placed in the center of symmetry in the principal glide plane of symmetry. A *Mg* position occupies this point. In pyrophyllite this position is vacant. Fig. 2 shows the unit cell of talc projected on the principal glide plane 010.

Summary.

Two talcs (Harford County and Vorwald) and two pyrophyllites (Graves Mountain and Mariposa County) were investigated with the powder method. The powder diagrams of the two specimens of each mineral are alike within the limits of error. The structures of the individual layers of talc and pyrophyllite agree with those predicted by Pauling. The stacking of the layers, however, is such that the two minerals belong to the monoclinic holohedral space group C_{2h}^6 instead of C_{2h}^3.

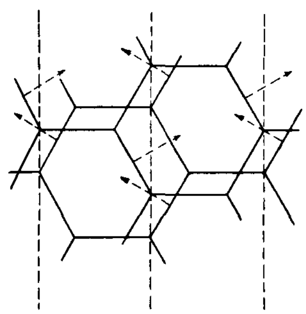

Fig. 1.

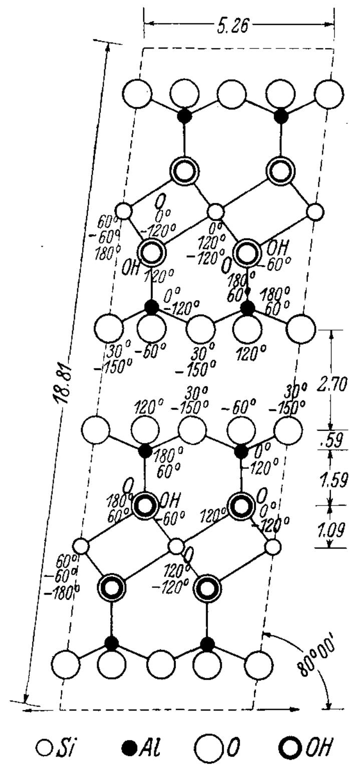

Fig. 2.

Fig. 1. Shifts of layers in talc and pyrophyllite. Dotted lines are principal glide planes of C_{2h}^{6}. Arrows indicate planes of symmetry in individual sheets.

Fig. 2. Unit cell of talc. The plane of the paper is the principal glide plane. y coordinates given in degrees.

Four molecules of $Mg_3Si_4O_{10}(OH)_2$ and $Al_2Si_4O_{10}(OH)_2$ respectively are combined in the unit cell. Other constants found are

	Talc	Pyrophyllite
$a_0 =$	5.26 $\pm$ .02 Å	5.14 $\pm$ .02 Å
$b_0 =$	9.10 $\pm$ .02	8.90 $\pm$ .02
$c_0 =$	18.81 $\pm$ .03	18.55 $\pm$ .03
$\beta =$	100°00 $\pm$ 5′	99°55 $\pm$ 5′
axial ratio	0.578 : 1.000 : 2.067	0.577 : 1.000 : 2.084
theoretical density	2.824	2.844

Received 3rd April 1934.