PYROPHYLLITE

1, 1TC, f-talc-pyrophyllite, s-pyrophyllite

Al[Si(2)O(5)](OH)

Triclinic C 1(-) Z = 4

R =0.06

20 .5 .1988

Ref.Str.:

Lee Y.H., Guggenheim S. (1981)
* Amer. Mineral., 66, 350-357

Reserv:

See U(jj) in the original,
Al(1.97)Fe(0.03)[Si(3.98)Al(0.02)]O(10)(OH)(2)

Initial data from BDM-file

Lattice parameters (cub. angs.,degr.):

a = 5.16 alpha = 91.18
b = 8.966 beta = 100.46
c = 9.34 gamma = 89.64

Unit cell volume (cub. angs.) = 424.84

Molar volume (cub.cm/mol.) = 63.97

Co-ordinates, thermal parameters, occupation for atomic positions:

NoP	x/a	y/b	z/c	B(j)	atom / occupation
1	0.4995	0.1671	0.9999	0.7	Al = 1.00
2	0.7449	0.997	0.2917	0.68	Si = 1.00
3	0.7595	0.3258	0.2923	0.7	Si = 1.00
4	0.6495	0.0018	0.1155	0.89	O = 1.00
5	0.7314	0.3079	0.1158	0.84	O = 1.00
6	0.2263	0.1927	0.1081	1.0	O = 1.00
7	0.0498	0.3891	0.3589	0.95	O = 1.00
8	0.7251	0.1637	0.3584	0.95	O = 1.00
9	0.5452	0.4426	0.3325	1.01	O = 1.00

Co-ordinates for all atomic positions :

No	NoP	x/a	y/b	z/c
1	1	0.4995	0.1671	0.9999
2	2	0.7449	0.997	0.2917
3	3	0.7595	0.3258	0.2923
4	4	0.6495	0.0018	0.1155
5	5	0.7314	0.3079	0.1158
6	6	0.2263	0.1927	0.1081
7	7	0.0498	0.3891	0.3589
8	8	0.7251	0.1637	0.3584
9	9	0.5452	0.4426	0.3325
10	1	0.5005	0.8329	0.0
11	2	0.2551	0.003	0.7083
12	3	0.2405	0.6742	0.7077
13	4	0.3505	0.9982	0.8845
14	5	0.2686	0.6921	0.8842
15	6	0.7737	0.8073	0.8919
16	7	0.9502	0.6109	0.6411
17	8	0.2749	0.8363	0.6416
18	9	0.4548	0.5574	0.6675
19	1	0.0005	0.3329	0.0
20	2	0.7551	0.503	0.7083
21	3	0.7405	0.1742	0.7077
22	4	0.8505	0.4982	0.8845
23	5	0.7686	0.1921	0.8842
24	6	0.2737	0.3073	0.8919
25	7	0.4502	0.1109	0.6411
26	8	0.7749	0.3363	0.6416
27	9	0.9548	0.0574	0.6675
28	1	0.9995	0.6671	0.0
29	2	0.2449	0.497	0.2917
30	3	0.2595	0.8258	0.2923
31	4	0.1495	0.5018	0.1155
32	5	0.2314	0.8079	0.1158
33	6	0.7263	0.6927	0.1081
34	7	0.5498	0.8891	0.3589
35	8	0.2251	0.6637	0.3584
36	9	0.0452	0.9426	0.3325

X-ray density (g/cm cub.) = 2.8

MU (1/cm) = 90.951 Mass attenuation coefficient (cm**2/g) = 32.483

Selected interatomic distances (cation-anion,anion-anion):

NoP	Atom	Rad.sph. (angs.)	C.N.	Distance (angs.)	NoP N.
1	Al	2.316	6		
				1.9256	4
				1.9211	5
				1.888	6
				1.9214	4
				1.925	5
				1.8878	6
2	Si	2.1	4		
				1.6312	4
				1.6175	8
				1.6154	7
				1.6024	9
3	Si	2.1	4		
				1.6331	5
				1.6159	7
				1.6138	8
				1.6065	9
4	O	3.264	10		
				2.7793	5
				2.7579	6
				2.6375	8
				2.4136	4
				2.8522	6
				2.9331	5
				2.7796	5
				2.7983	6
				2.6419	7
				2.6621	9
5	O	3.264	10		
				2.7793	4
				2.7611	6
				2.7978	6
				2.6414	7
				2.6372	8
				2.6588	9
				2.9331	4
				2.4186	5
				2.8561	6

				2.7796	4
6	0		3.264	9	
				2.7579	4
				2.7978	5
				2.7611	5
				3.1626	7
				3.1606	8
				2.8522	4
				2.8561	5
				2.3369	6
				2.7983	4
7	0		3.264	8	
				2.6414	5
				3.1626	6
				2.6326	8
				2.6598	9
				2.6127	9
				3.26	8
				2.6419	4
				2.6287	8
8	0		3.264	10	
				2.6375	4
				2.6372	5
				3.1606	6
				2.6326	7
				2.6622	9
				3.26	7
				3.0078	8
				3.083	9
				2.6287	7
				2.6078	9
9	0		3.264	7	
				2.6588	5
				2.6127	7
				2.6598	7
				2.6622	8
				3.083	8
				2.6621	4
				2.6078	8