KAOLINITE

4, at 1.5' K, f-kaolinite-halloysite, sf-kaolinite

Al(2)Si(2)O(5)(OH)(4)

Triclinic C 1 Z = 2

R =0.0178

3 .6 .1998

Ref.Str.:

Bish D.L. (1993)
* Clays & Clay Minerals, 41, 738-744

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

a = 5.1535 alpha = 91.93
b = 8.9419 beta = 105.04
c = 7.3906 gamma = 89.8

Unit cell volume (cub. angs.) = 328.71

Molar volume (cub.cm/mol.) = 99.0

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

NoP	x/a	y/b	z/c	B(j)	atom	/ occupation
1	0.049	0.3482	0.3168	0.04	O	= 1.00
2	0.113	0.6599	0.3188	0.04	O	= 1.00
3	0.0	0.5	0.0	0.04	O	= 1.00
4	0.204	0.2291	0.03	0.04	O	= 1.00
5	0.197	0.7641	0.001	0.04	O	= 1.00
6	0.05	0.971	0.325	0.04	OH	= 1.00
7	0.96	0.1658	0.607	0.04	OH	= 1.00
8	0.037	0.4726	0.6046	0.04	OH	= 1.00
9	0.038	0.8592	0.609	0.04	OH	= 1.00
10	0.289	0.4966	0.466	0.04	Al	= 1.00
11	0.793	0.3288	0.465	0.04	Al	= 1.00
12	0.989	0.3395	0.0906	0.04	Si	= 1.00
13	0.507	0.1665	0.0938	0.04	Si	= 1.00
14	0.145	0.0651	0.326	0.07	H	= 1.00
15	0.063	0.1638	0.739	0.05	H	= 1.00
16	0.036	0.5057	0.732	0.06	H	= 1.00
17	0.534	0.3154	0.728	0.05	H	= 1.00

Co-ordinates for all atomic positions :

No	NoP	x/a	y/b	z/c
1	1	0.049	0.3482	0.3168
2	2	0.113	0.6599	0.3188
3	3	0.0	0.5	0.0
4	4	0.204	0.2291	0.03
5	5	0.197	0.7641	0.001
6	6	0.05	0.971	0.325
7	7	0.96	0.1658	0.607
8	8	0.037	0.4726	0.6046
9	9	0.038	0.8592	0.609
10	10	0.289	0.4966	0.466
11	11	0.793	0.3288	0.465
12	12	0.989	0.3395	0.0906
13	13	0.507	0.1665	0.0938
14	14	0.145	0.0651	0.326
15	15	0.063	0.1638	0.739
16	16	0.036	0.5057	0.732
17	17	0.534	0.3154	0.728
18	1	0.549	0.8482	0.3168
19	2	0.613	0.1599	0.3188
20	3	0.5	0.0	0.0
21	4	0.704	0.7291	0.03
22	5	0.697	0.2641	0.001
23	6	0.55	0.471	0.325
24	7	0.46	0.6658	0.607
25	8	0.537	0.9726	0.6046
26	9	0.538	0.3592	0.609
27	10	0.789	0.9966	0.466
28	11	0.293	0.8288	0.465
29	12	0.489	0.8395	0.0906
30	13	0.007	0.6665	0.0938
31	14	0.645	0.5651	0.326
32	15	0.563	0.6638	0.739
33	16	0.536	0.0057	0.732
34	17	0.034	0.8154	0.728

X-ray density (g/cm cub.) = 2.65

MU (1/cm) = 78.08 Mass attenuation coefficient (cm**2/g) = 29.485

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

NoP	Atom	Rad.sph. (angs.)	C.N.	Distance (angs.)	NoP N.
1	O	3.312	10		
				2.8069	2
				2.7004	3
				2.6432	4
				2.8673	7
				2.382	8
				2.816	2
				2.6452	5
				2.7946	6
				2.8069	6
				2.8611	9
2	O	3.312	10		
				2.8069	1
				2.6461	3
				2.6926	5
				2.7998	6
				2.8446	8
				2.845	9
				2.816	1
				2.6693	4
				2.8021	6
				2.3986	7
3	O	3.312	8		
				2.7004	1
				2.6461	2
				2.6305	4
				2.5729	5
				2.9794	8
				2.5876	4
				2.6303	5
				3.2207	6
4	O	3.312	8		
				2.6432	1
				2.6305	3
				3.0855	7
				2.6693	2
				2.5876	3
				2.6252	5

				2.5843	5
				3.2099	6
5	O	3.312	8		
				2.6926	2
				2.5729	3
				3.2194	6
				2.9523	9
				2.6452	1
				2.6303	3
				2.5843	4
				2.6252	4
6	OH	3.36	10		
				2.7998	2
				3.2194	5
				2.8009	7
				2.3702	9
				2.8069	1
				2.7946	1
				2.8021	2
				3.2207	3
				3.2099	4
				2.8062	8
7	OH	3.36	8		
				2.8673	1
				3.0855	4
				2.8009	6
				2.7746	8
				2.7695	9
				2.3986	2
				2.7824	8
				2.7765	9
8	OH	3.36	8		
				2.382	1
				2.8446	2
				2.9794	3
				2.7746	7
				2.8062	6
				2.7824	7
				2.7633	9
				2.7761	9
9	OH	3.36	8		
				2.845	2
				2.9523	5
				2.3702	6
				2.7695	7
				2.8611	1
				2.7765	7
				2.7761	8
				2.7633	8

10	Al	2.364	6		
				1.9266	1
				1.9296	2
				1.868	8
				1.9123	6
				1.8916	7
				1.9092	9
11	Al	2.364	6		
				1.9326	1
				1.8951	7
				1.8836	8
				1.9206	2
				1.9131	6
				1.9072	9
12	Si	2.148	4		
				1.6185	1
				1.6113	3
				1.6196	4
				1.6178	5
13	Si	2.148	4		
				1.6135	4
				1.613	2
				1.6176	3
				1.608	5
14	H	1.68	1		
				0.9738	6
15	H	1.68	1		
				0.9829	7
16	H	1.68	1		
				0.9787	8
17	H	1.68	1		
				0.9798	9