TALC

1, f-talc-pyrophyllite, s-talc

Mg(3)[Si(4)O(10)](OH)(2)

Triclinic P 1(-) Z = 2

P1(-)

27 .5 .1988

Ref.Str.:

Perdikatsis B., Burziaff H. (1981)

* Z. Kristallogr., 156, 177-186

Initial data from BDM-file

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

a = 5.291 alpha = 98.68
b = 9.46 beta = 119.9
c = 5.29 gamma = 85.27

Unit cell volume (cub. angs.) = 226.9

Molar volume (cub.cm/mol.) = 68.34

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

NoP	x/a	y/b	z/c	B(j)	atom / occupation
1	0.0052	0.7093	0.2573	0.0	Si = 1.00
2	0.6714	0.7089	0.59	0.0	Si = 1.00
3	0.0	0.0	0.0	0.0	Mg = 1.00
4	0.6666	0.0001	0.3332	0.0	Mg = 1.00
5	0.6688	0.8824	0.6453	0.0	O = 1.00
6	0.3348	0.8874	0.9704	0.0	O = 1.00
7	0.0024	0.8824	0.3032	0.0	O = 1.00
8	0.8574	0.6519	0.9088	0.0	O = 1.00
9	0.8218	0.6506	0.3907	0.0	O = 1.00
10	0.3398	0.6516	0.427	0.0	O = 1.00
11	0.338	0.797	0.95	0.0	H = 1.00

Co-ordinates for all atomic positions :

No	NoP	x/a	y/b	z/c
1	1	0.0052	0.7093	0.2573
2	2	0.6714	0.7089	0.59
3	3	0.0	0.0	0.0
4	4	0.6666	0.0001	0.3332
5	5	0.6688	0.8824	0.6453
6	6	0.3348	0.8874	0.9704
7	7	0.0024	0.8824	0.3032
8	8	0.8574	0.6519	0.9088
9	9	0.8218	0.6506	0.3907
10	10	0.3398	0.6516	0.427
11	11	0.338	0.797	0.95
12	1	0.9948	0.2907	0.7427
13	2	0.3286	0.2911	0.41
14	4	0.3334	0.0	0.6668
15	5	0.3312	0.1176	0.3547
16	6	0.6652	0.1126	0.0296
17	7	0.9976	0.1176	0.6968
18	8	0.1426	0.3481	0.0912
19	9	0.1782	0.3494	0.6093
20	10	0.6602	0.3484	0.573
21	11	0.662	0.203	0.05

X-ray density (g/cm cub.) = 2.77

MU (1/cm) = 86.558 Mass attenuation coefficient (cm**2/g) = 31.195

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

NoP	Atom	Rad.sph. (angs.)	C.N.	Distance (angs.)	NoP N.
1	Si	2.1	4		
				1.619	7
				1.6235	8
				1.6238	9
				1.6254	10
2	Si	2.1	4		
				1.6231	5
				1.6237	8
				1.6239	9
				1.6197	10

3	Mg	2.52	6		
				2.0597	5
				2.0523	6
				2.08	7
				2.0597	5
				2.0523	6
				2.08	7
4	Mg	2.52	6		
				2.121	5
				2.0576	6
				2.0789	7
				2.0584	5
				2.0531	6
				2.0785	7
5	O	3.264	12		
				3.0558	6
				3.0124	6
				3.1014	6
				3.0172	7
				3.0944	7
				3.0571	7
				2.6202	8
				2.6797	9
				2.6443	10
				2.8537	5
				2.7516	6
				2.8345	7
6	O	3.264	9		
				3.1014	5
				3.0124	5
				3.0558	5
				3.0621	7
				3.053	7
				3.0541	7
				2.7516	5
				2.7495	6
				2.785	7
7	O	3.264	12		
				3.0571	5
				3.0944	5
				3.0172	5
				3.0541	6
				3.053	6
				3.0621	6
				2.6464	8
				2.6512	9
				2.6469	10
				2.8345	5
				2.785	6

				2.8163	7
8	O	3.264	8		
				2.6202	5
				2.6464	7
				2.6501	9
				2.6501	9
				2.6561	10
				2.6526	10
				3.184	8
				3.0975	10
9	O	3.264	6		
				2.6797	5
				2.6512	7
				2.6501	8
				2.6501	8
				2.651	10
				2.6504	10
10	O	3.264	8		
				2.6443	5
				2.6469	7
				2.6526	8
				2.6561	8
				2.6504	9
				2.651	9
				3.0975	8
				3.2029	10
11	H	1.632	1		
				0.8455	6