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The crystal structure of lizardite 1*T*: hydrogen bonds and polytypism

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Abstract

The occurence of lizardite 1*T* from Val Sissone, Italy, is reported. Electron microprobe analysis leads to the doubled unit cell content

$$(Mg_{5.58}Fe^{2+}_{0.08}Fe^{3+}_{0.20}Al_{0.14})\ (Si_{3.66}Al_{0.34})O_{10.00}(OH)_{8.00}.$$

The unit cell parameters are $a = 5.332(3)$Å, $c = 7.233(4)$Å, space group is $P31m$.

The crystal structure has been refined, using 209 symmetry independent reflections, to $R = 0.031$. The refined model is not far from the idealized geometry of the serpentine layer. The ditrigonal distortion of the six-membered tetrahedral ring is small ($\alpha = -3.5°$). No buckling of the brucite-like sheet is observed.

The occurrence of both negative and positive α values in serpentine minerals is explained on the basis of stacking sequence and hydrogen bonds. Namely, the best hydrogen bond system is attained by rotation of the bridging oxygens belonging to the tetrahedral sheet. The direction of rotation depends on the way in which subsequent layers are stacked one upon the other. The substitution of trivalent atoms for magnesium and silicon leads to stronger hydrogen bonding between adjacent layers, thus promoting the formation of flat-layer structures and increasing thermal stability.

Introduction

The well-known classification of the serpentine minerals was developed by Whittaker and Zussmann (1956). The scheme is based on the recognition of cylindrical layers in chrysotile, corrugated layers in antigorite, and flat layers in lizardite. A recent review of the crystal structure of the serpentine minerals was given by Wicks and Whittaker (1975). The most serious handicap to full understanding of the serpentine structures is the low degree of three-dimensional order present in these minerals. For instance, the previous two-dimensional determinations of the crystal structure of lizardite, by Rucklidge and Zussman (1965) and by Krstanovic (1968), led to discrepancy factors of 18 percent and 19 percent respectively, in spite of the fact the flat-layer lizardite structure would seem to be the most promising for X-ray diffraction analysis.

Lizardite from Kennack Cove (Rucklidge and Zussman, 1965) is composed of domains of 1*T* and disordered 2*H* polytypes. Lizardite from Radusa Mine (Krstanovic, 1968) is composed of the 1*T* polytype. According to Rucklidge and Zussman (1965), the average crystal structure has trigonal symmetry, but Krstanovic (1968) refined his model in the space group *Cm*. Subsequently, Wicks and Whittaker (1975), in discussing Krstanovic's refinement, stated that lizardite 1*T* "is in fact orthorhombic and only pseudo-trigonal".

Wicks and Whittaker (1975) and Krstanovic (1980) have discussed the distortions of both the tetrahedral and the octahedral sheets of a very pure lizardite 1*T* with limited substitutions for silicon or magnesium. According to these authors, the composition of lizardite 1*T* from Radusa Mine results in a large misfit between the tetrahedral and octahedral sheets, and produces shifts of the atoms away from the ideal positions. In particular, they noted buckling of the plane of the magnesium atoms and various shifts, along [001], of the oxygen, silicon and magnesium atoms. In this present paper, I report a more regular model for the crystal structure of lizardite 1*T* from Val Sissone, Italy, that contains significant aluminum and iron substitution. The structure is not very different from the idealized geometry of the serpentine layer and was refined using diffraction data obtained on euhedral crystals of lizardite 1*T*. The different composition of the Val Sissone lizardite 1*T*, with its different structural constraints, limits comparison with the lizardite 1*T*

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Neilson 3961 AM-82-201 Table 4

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LIZARDITE

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	0	-10	12	12	3	3	-5	16	16	1	2	-2	10	11	3	3	0	29	29	1	5	2	6	6
1	1	-9	22	21	0	4	-5	9	9	2	2	-2	22	22	1	4	0	10	10	2	5	2	10	10
0	2	-9	7	8	1	4	-5	7	7	0	3	-2	19	19	3	4	0	4	4	0	6	2	14	14
0	0	-8	22	22	2	4	-5	6	7	1	3	-2	7	8	0	5	0	6	6	0	0	3	20	20
0	1	-8	2	3	0	0	-4	20	20	2	3	-2	7	7	1	5	0	6	6	0	1	3	9	10
1	1	-8	15	15	0	1	-4	8	7	3	3	-2	12	12	2	5	0	6	6	1	1	3	13	13
0	2	-8	8	7	1	1	-4	31	31	0	4	-2	6	6	0	6	0	28	28	0	2	3	13	13
0	3	-8	20	20	0	2	-4	13	13	1	4	-2	17	17	0	1	1	17	17	1	2	3	7	7
0	0	-7	18	19	1	2	-4	6	7	2	4	-2	5	4	1	1	1	19	20	2	2	3	38	38
0	1	-7	2	3	2	2	-4	35	35	3	4	-2	5	5	0	2	1	8	8	0	3	3	15	14
1	1	-7	6	7	0	3	-4	9	10	0	5	-2	6	5	1	2	1	11	11	1	3	3	7	7
0	2	-7	9	9	1	3	-4	4	5	1	5	-2	5	5	2	2	1	45	45	2	3	3	6	5
1	2	-7	3	3	2	3	-4	5	5	2	5	-2	10	10	0	3	1	26	26	3	3	3	10	10
2	2	-7	10	10	3	3	-4	7	7	0	6	-2	14	14	1	3	1	10	10	0	4	3	7	7
0	3	-7	16	15	0	4	-4	8	8	0	1	-1	17	17	2	3	1	6	7	1	4	3	5	5
0	4	-7	6	7	1	4	-4	18	18	1	1	-1	55	55	3	3	1	13	13	2	4	3	5	5
0	0	-6	24	24	2	4	-4	6	6	0	2	-1	8	7	1	4	1	10	10	0	5	3	5	5
0	1	-6	4	4	0	0	-3	20	20	1	2	-1	12	11	0	5	1	6	6	0	6	3	8	8
1	1	-6	18	18	0	1	-3	10	10	2	2	-1	22	22	1	5	1	6	6	0	0	4	20	20
0	2	-6	12	12	1	1	-3	45	45	0	3	-1	27	26	2	5	1	19	18	0	1	4	7	7
1	2	-6	4	4	0	2	-3	13	13	1	3	-1	9	9	3	6	1	9	8	1	1	4	43	44
2	2	-6	11	11	1	2	-3	9	8	2	3	-1	8	8	0	0	2	48	48	0	2	4	13	13
0	3	-6	20	20	2	2	-3	6	7	3	3	-1	14	14	0	1	2	14	14	1	2	4	6	5
1	3	-6	5	5	0	3	-3	15	14	1	4	-1	27	27	1	1	2	19	19	2	2	4	16	16
3	3	-6	13	13	1	3	-3	6	5	0	5	-1	7	6	0	2	2	11	11	0	3	4	9	10
0	4	-6	9	8	2	3	-3	5	6	1	5	-1	6	5	1	2	2	9	10	1	3	4	6	6
1	4	-6	11	11	3	3	-3	12	11	2	5	-1	7	7	2	2	2	15	15	3	3	4	6	5
0	0	-5	24	24	0	4	-3	7	7	0	6	-1	8	8	0	3	2	19	19	0	4	4	7	8
0	1	-5	6	6	1	4	-3	24	24	0	1	0	18	18	1	3	2	9	9	1	4	4	26	26
1	1	-5	14	14	2	4	-3	6	5	1	1	0	11	10	2	3	2	6	7	2	4	4	6	6
0	2	-5	14	14	0	5	-3	4	5	0	2	0	7	7	3	3	2	12	12	1	5	4	5	4
1	2	-5	5	6	0	6	-3	8	8	1	2	0	12	12	0	4	2	6	6	0	0	5	24	24
2	2	-5	22	22	0	0	-2	48	48	2	2	0	19	19	1	4	2	16	16	0	1	5	5	6
0	3	-5	24	24	0	1	-2	14	14	0	3	0	54	54	2	4	2	4	4	1	1	5	37	38
1	3	-5	3	3	1	1	-2	44	43	1	3	0	9	9	3	4	2	5	4	0	2	5	13	14
2	3	-5	3	4	0	2	-2	11	11	2	3	0	7	7	0	5	2	5	5	2	2	5	9	9

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Table 4

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	3	5	23	24	0	0	6	24	24	3	3	6	14	14	2	2	7	6	5	2	2	8	7	8
1	3	5	4	5	0	1	6	5	4	0	4	6	8	8	0	3	7	14	15	0	3	8	20	19
3	3	5	14	13	1	1	6	12	11	1	4	6	8	8	1	4	7	10	11	1	1	9	12	11
0	4	5	8	9	0	2	6	11	12	0	0	7	15	19	0	0	8	21	22	0	2	9	5	6
1	4	5	21	22	2	2	6	9	9	1	1	7	17	18	1	1	8	7	6	0	0	10	12	12
2	4	5	7	6	0	3	6	20	20	0	2	7	9	9	0	2	8	7	7					