The crystal structure of a new (*m* = 16) antigorite polysome

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In a previous report [1] we briefly described the "state of the art" on the crystal structure of the mineral antigorite (s. also [2]), the difficulties to obtain reliable structural data with conventional sources, and some preliminary results of the collection carried out in the past 2003 at the Desy F1 line.

Since then, our efforts have being paid on the A11 sample, which showed a metrically triclinic cell (a = 41.10; b = 9.26; c = 7.26 Å; α = 90; β = 88.6; γ = 83.5°) that was transformed to the monoclinic setting (a = 81.66; b = 9.26; c = 7.26; β = 91.41°). After structure solution with the SIR97 program [3], we isotropically refined the structure in the *C*2/*m* *S.G.* down to the provisional $R_{obs} \approx 13\%$, using SHELX97 [4]. Selected collection and crystal data are summarized in Table 1.

Table 1. Collection and crystal data

λ = 0.7107 Å
Refls. collected / unique: 16479 / 4033 [R_{int} = 0.064]
Crystal size: 160 x 60 x 30 mμ
Ideal formula: $Mg_{45}Si_{32}O_{80}(OH)_{58}$
S.G. = *C*2/*m*
A = 81.66, *b* = 9.26, *c* = 7.26 Å, *b* = 91.41°
93 unique atoms (546 in the cell)
Data / restraints / parameters: 16479 / 242 / 325
Provisional *R*1 / observed [I > 2s(I)] = 0.1289 / 5,950

The *m* = 16 antigorite structure preserves the basic structural features of the well known *m* = 17 polysome [2]: a 6-membered tetrahedral (T) Si-O sheet links a continuous, wavy octahedral (O) Mg-O sheet on the concave side, inverting polarities at reversal lines through alternating 6-membered and 8-membered tetrahedral units. The *C*-centred cell derives from the ½ *b* offset of any subsequent 8-reversal (Fig. 1). This structure therefore improves and supersedes the previous TEM model [5].

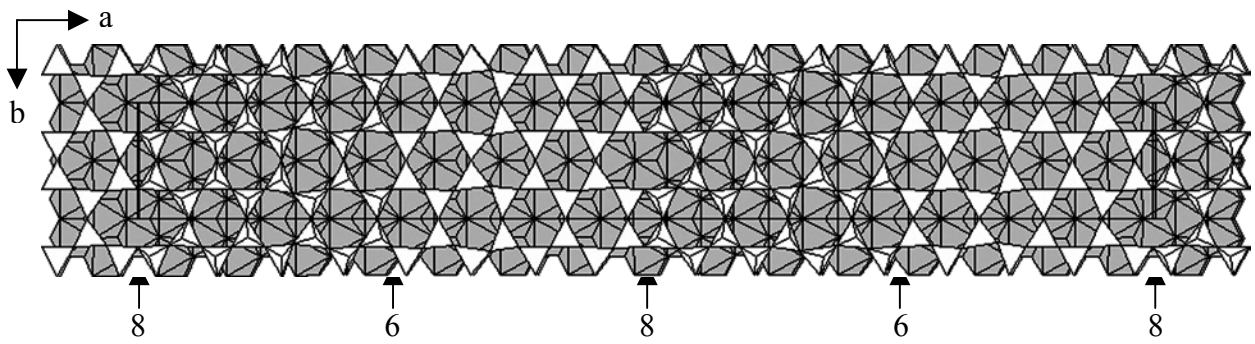

Fig. 1. Antigorite *m* = 16 polysome as seen down [001].

As regard the bond geometry, the mean Si-O distance of the *m* = 16 polysome (1.633 Å) matches those of the *m* = 17 polysome (1.637 Å) and of lizardite 1*T* (1.64-1.66 Å) [6]. In all these structures the apical Si-O distances are shorter than the basal ones.

The mean Mg-O distance of the *m* = 16 polysome (2.090 Å) matches the one of the *m* = 17 polysome (2.088 Å). Both are slightly longer than those of lizardite 1*T* (2.07 Å). In both polysomes, the outer Mg-O distances are slightly shorter than the inner ones, like in lizardite. Therefore, the two antigorite polysomes have extremely similar Mg-polyhedra, very similar also to the Mg-polyhedra of lizardite.

The two antigorite polysomes have very similar T-sheet and O-sheet thicknesses, very close to the ones of lizardite too (2.22 and 2.11, respectively). At reversal lines, the thickness of the antigorite TO layer is slightly larger than between reversals.

Deviations from the “hexagonality” occur in the 6-membered tetrahedral sheet of both antigorite polysomes, with very close average values and ranges of variation along the wave. Higher deviations occur near reversal lines. Even with some differences, similar deviations occur also in lizardite [6, 7].

Therefore, no unique features exist for antigorite with respect the other serpentine polymorphs as far as the nearest neighbors interactions are concerned, making antigorite an example of “supramolecular crystallography”, in which many physical-chemical properties can be inferred from the knowledge of the basic building blocks, in the present case the individual TO module.

References

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