

Crystal Structure Refinement of Palygorskite of the Ventzia Basin, Western Macedonia/Greece, by the Rietveld Method.

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The mineralogy of the palygorskite and Mg-Fe-smectite clay deposits, of the Ventzia basin, western Macedonia/Greece, was studied by Kastritis et al. (2003). It is a sedimentary ore deposit of palygorskite and Mg-Fe smectite clays.

In this study the crystal structure of the palygorskite was investigated by x-ray powder diffraction and Rietveld refinement techniques. The data collection was performed by a D8 Advance x-ray powder diffractometer, from BRUKER, with copper radiation and the LynxEye detector. For the Rietveld refinement the software TOPAS 4 was used.

Qualitatively the investigated palygorskite sample consists of two palygorskite polymorphs and minor quantity of quartz. For the Rietveld refinement the monoclinic (C2/m) and the orthorhombic (Pbmn) crystal structures of palygorskite were used, Chiari et. al. (2003), Giustetto et al. (2004).

The refined cell parameters and the refinement details for the two polymorphs are:

	M Palygorskite	O Palygorskite	
Space group	C2/m	Pbmn	
a (Å)	13.296(5)	12.940(5)	
b (Å)	17.817(5)	17.865(5)	
c (Å)	5.264 (3)	5.247 (3)	
β (°)	106.38 (3)	90	
V (Å ³)	1188.7	1212.9	
Quantity	17.2%	80.0%	(Quartz 2.8%)
Rp		4.1	
Rwp		4.9	5.5
R- Bragg	6.1		

According to Gueven et al. (1992) from the three octahedral positions, M1 is vacant, M2 is occupied by Mg and M3 is occupied by Al.

The mineral, formula based to the Rietveld refinement results and microprobe analysis, is:



The total occupation number of the octahedral sheet is 4.05 and the ratio R^{2+}/R^{3+} is 0.98.

The relation between lattice parameters and octahedral sheet occupancy is similar as reported by Suarez et. Al. 2007.

References

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