

Implications for the Nomenclature of p-p Hydropyroxenoids: the Crystal Structure of Marsturite from the Molinello mine, Liguria, Italy

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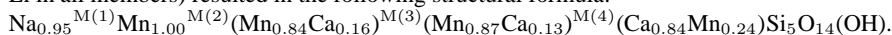
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The previously unstudied crystal structure of the p-p (pectolite-pyroxene) hydropyroxenoid marsturite, originally described from Franklin, New Jersey, USA (Peacor et al., 1978), has been determined using a sample from the Molinello mine, Val Graveglia, Liguria, Italy (sample in collection of Stift Melk, Melk, Austria).

Refinement of the single-crystal intensity data (Mo-K α X-radiation, CCD area detector, RT, $R(F) = 5.5\%$) gave triclinic space-group symmetry $P-1$ (no. 2), with $a = 6.771(1)$, $b = 7.697(2)$, $c = 11.720(2)$ Å, $\alpha = 106.83(3)$, $\beta = 92.40(3)$, $\gamma = 94.41(3)^\circ$, $V = 581.6(2)$ Å³.

The results confirm that marsturite belongs to a group of four isotypic silicate minerals, viz. nambulite - (Li,Na)Mn₄Si₅O₁₄(OH) (Narita et al., 1975), natronambulite - NaMn₄Si₅O₁₄(OH) (Matsubara et al., 1985), lithiomarsturite - LiCa₂Mn₂Si₅O₁₄(OH) (Peacor et al., 1990) and marsturite - NaCaMn₃Si₅O₁₄(OH). Their topology is based on infinite silicate chains with a repeat unit of five SiO₄ tetrahedra (*finferketten*) which are connected to polyhedral bands of edge-sharing $Met^{2+}O_6$ ($Met = Mn, Ca$; minor Fe, Mg) octahedra and CaO₇ polyhedra. Both chains and bands run along [011]. The [6]- to [8]-coordinated Li⁺/Na⁺ cations occupy voids.

Refinement of the occupancies of the four divalent metal sites M(1)-M(4) and the M(5) site (occupied by either Na or Li in all members) resulted in the following structural formula:



The bulk composition is very similar to the one reported for the type material (Peacor et al., 1978) and to marsturite from Molinello EMP-analysed by Palenzona (1987). The dominance of Ca on the M(4) site is in good agreement with predictions of Peacor et al. (1990) and crystal-structure data reported for the other members. The inferred preference of Ca also for the M(2) site is confirmed as well. The maximum Ca:Mn ratio in these hydropyroxenoids appears to be 1:1. Thus, at least one hypothetical end-member is awaiting its discovery in nature: NaCa₂Mn₂Si₅O₁₄(OH), with Ca dominant on both M(2) and M(4).

The very strong hydrogen bond (ca. 2.5 Å) in these hydropyroxenoids will also be discussed.

References

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