

Intermediate scapolite: crystal chemistry, structure and behavior at non-ambient (*P,T*)-conditions

Lotti P.*¹, Gatta G.D.¹, Gigli L.², Merlini M.¹, Comboni D.¹ & Krüger H.³

¹ Dipartimento di Scienze della Terra, Università degli Studi di Milano

² Elettra Sincrotrone Trieste S.c.P.A.

³ Institut für Mineralogie und Petrographie, Universität Innsbruck

* Corresponding email: paolo.lotti@unimi.it

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Scapolites, general formula $M_4T_{12}O_{24}A$, are important minerals in metamorphic rocks, ranging from the greenschists to the amphibolite facies, where can act as hosts for volatiles (mainly Cl⁻, CO₃²⁻ and SO₄²⁻ anions). From the crystal-chemical point of view, they represent a complex group of minerals, for which three end members have been described: marialite (Na₄Al₃Si₉O₂₄Cl), meionite (Ca₄Al₆Si₆O₂₄CO₃) and silvialite (Ca₄Al₆Si₆O₂₄SO₄). Along the marialite-meionite joint, complex substitution mechanisms govern the occurrence of three binary solid solutions (Sokolova & Hawthorne, 2008), which are coupled with intriguing crystallographic features. In fact, in the literature, the members close to the marialite and meionite sides are reported to crystallize in the *I4/m* space group, whereas the intermediate members are always reported to share the *P4₂/n* space group.

In this work, a gem-quality transparent single-crystal of intermediate scapolite ((Na_{1.86}Ca_{1.86}K_{0.23}Fe_{0.01}) (Al_{4.36}Si_{7.64})O₂₄[Cl_{0.48}(CO₃)_{0.48}(SO₄)_{0.01}]) from Madagascar has been investigated by means of both conventional lab and synchrotron X-ray diffraction. Interestingly, all the experimental X-ray diffraction datasets show the occurrence of systematic extinctions compatible with an *I*-centered lattice, which is in contrast to what expected for an intermediate scapolite member.

The high-pressure and high-temperature behaviors of the same intermediate sample of scapolite have also been investigated by means of in situ powder and single-crystal X-ray diffraction, using conventional X-ray sources, at the University of Innsbruck (HT-SCXRD), or synchrotron facilities, at Elettra (Trieste, HT-PXRD) and at ESRF (Grenoble, HP-SCXRD).

The high-*P* evolution of the unit-cell volume of scapolite has been fitted by a III-order Birch-Murnaghan equation of state, which yielded a refined bulk modulus of 70(2) GPa ($\beta_{V0} = 0.0143(4) \text{ GPa}^{-1}$). A comparison with the high-pressure behavior of three further members belonging to the marialite-meionite joint (Hazen & Sharp, 1988; Comodi et al., 1990) confirms the control played by the crystal chemistry on the bulk compressibility: at a first approximation, the bulk modulus linearly increases from marialite to meionite. In addition, a displacive phase transition from the *I4/m* toward a triclinic polymorph was found to occur at 9.87 GPa.

Preliminary analysis of the high-temperature data revealed a significant anisotropic thermal expansion, which is almost exclusively accommodated in the plane perpendicular to the tetragonal axis, i.e. (*hk0*).

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