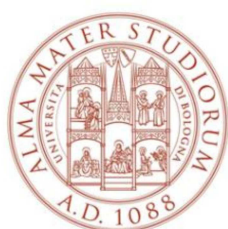
The logo for the 5th AIC Meeting features a large blue number '5' on the left. To its right is a blue molecular structure of a dodecahedron. Further right, the letters 'A I C' are arranged in a grid pattern, with a 'th' in a smaller font between the 'I' and 'C'. To the right of the grid is a blue line graph with several peaks of varying heights, resembling a chromatogram or mass spectrum.

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Book of abstracts



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(*P,T*)-behavior of an intermediate scapolite of unusual *I4/m* symmetry

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Scapolites are a group of open-framework aluminosilicates with general formula $M_4T_{12}O_{24}A$, where M are monovalent or divalent cations (usually Na, Ca and minor K), T are trivalent or tetravalent cations (mostly Al and Si) in tetrahedral coordination, and A are anionic elements or groups such as Cl, CO₃ and SO₄. Samples with a composition closer to the Na₄Al₃Si₉O₂₄Cl and Ca₄Al₆Si₆O₂₄CO₃ end-members are usually reported to crystallize with a structure described in the *I4/m* space group, whereas intermediate members are reported to show a *P4₂/n* symmetry. Scapolites are usually formed under metamorphic conditions in the presence of fluids, but are also reported as constituents of upper mantle xenoliths [1, 2]. Scapolites form a complex non-binary solid solution as a function of the (NaCl)-(CaCO₃)-(CaSO₄) substitutions, which couples with Al-Si re-arrangements [3, 4]. The variable crystal chemistry and symmetry of these minerals influences their elastic and structural response to pressure and temperature variations and, consequently, their stability fields. In this study, we have investigated the behavior of an intermediate scapolite of the composition (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}] and its unusual symmetry *I4/m*, by means of in situ X-ray and neutron diffraction at high-*T* (from -100 to +1000 °C), high-*P* (up to 17.8 GPa) and combined high-*T* and *P* (up to 650 °C and 16 GPa). Experimental data show that the unusual *I*-centered lattice is always preserved, whereas a phase transition towards a triclinic polymorph, that can be described according to an unconventional *I*-1 symmetry, was found to occur at 9-10 GPa, with a modest influence from temperature. The deformation mechanisms, acting at the atomic scale, that lead to the structural instability and phase transition have been described on the basis of a series of single-crystal structure refinements. A comparison with data from literature allows to model the elastic response of scapolites as a function of their crystal chemistry, whereas a model of the thermo-elastic behavior is less straightforward on the basis of the available data, suggesting that a thorough re-investigation of the thermal behavior of the complex scapolite solid solution is desirable.

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