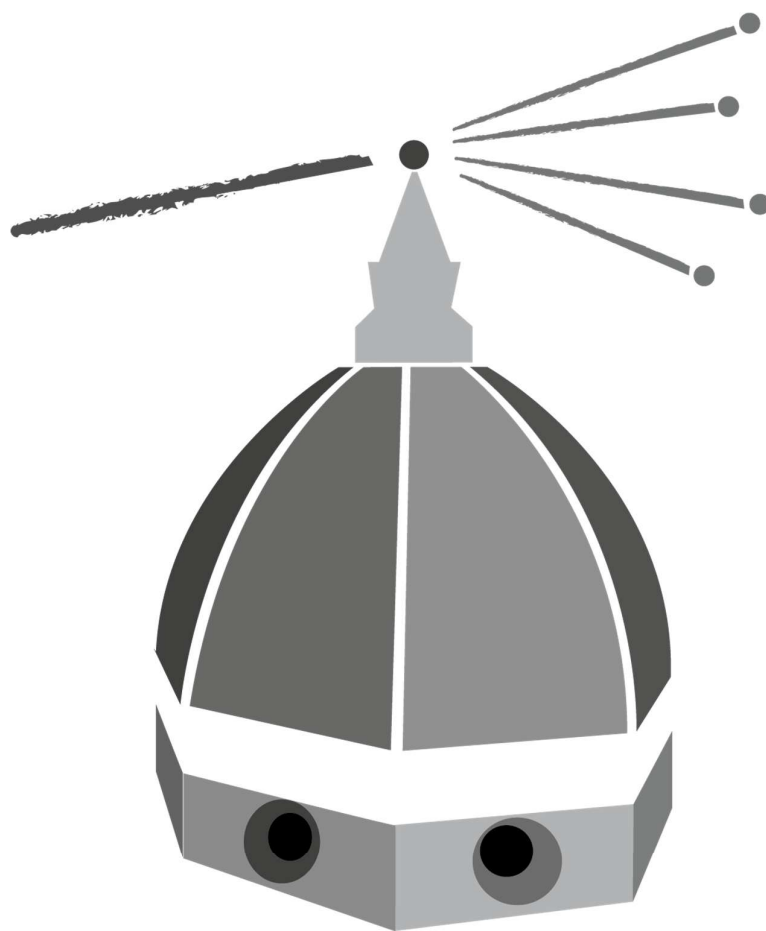


51st Meeting of the Italian Association of Crystallography



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Polytypism and swelling properties of 11.5 Å phase: a major water carrier to the mantle transition zone

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The understanding of the deep water cycle is crucial to assess the mechanisms behind large scale geological processes. In subduction zones, the water transport occurs through mineralogical reactions that involve the destabilization of water-bearing phases. In the last thirty years, high-pressure and high-temperature syntheses revealed the existence of new complex silicates that form after the destabilization of known hydrous minerals (e.g., antigorite, chlorite) and could play a crucial role in the transport and release of water in the mantle [1]. To understand the behaviour of these phases under mantle conditions and the dehydration mechanisms involved, crystallographic information and thermo-elastic studies are needed. Among these phases (Figure 1), the 11.5 Å phase [2], with chemical formula $\text{Mg}_6\text{Al}(\text{SiO}_4)_2(\text{OH})_7$, has a wide stability field along with the 23 Å phase [3]. The two phases share the same chemical formula, but their structural relation remained an open question. The 11.5 Å phase structure has been obtained with standard precession-assisted electron diffraction tomography (PEDT), revealing a layered structure consisting of TOT groups and double di-octahedral layers of face-sharing octahedra, with unit cell parameters $a = 9.012(1)\text{Å}$ $b = 5.201(1)\text{Å}$ $c = 23.202(5)\text{Å}$ $\beta = 97.8(1)^\circ$ and space group $C2/c$ [4], while for the 23 Å phase there is no structural information. We performed multi-anvil syntheses at different pressure-temperature conditions starting from natural chlorites with variable composition to obtain chemical and crystallographic information in this system. Single-crystal X-ray diffraction (SC-XRD) allowed for the first structural solution of the 23 Å phase, which resulted in an orthorhombic pseudo-hexagonal polytype of the 11.5 Å phase, with space group $Cmcm$ and unit cell parameters $a = 8.9783(3)\text{Å}$ $b = 5.2018(2)\text{Å}$ $c = 22.9982(8)\text{Å}$. We also report SC-XRD thermo-elastic studies on both polytypes, that revealed an interesting behaviour. A single crystal to single crystal phase transition at 400°C revealed a 5% volume increase upon partial dehydration, associated with an unpacking of the double Mg-octahedral layers. The energy release associated with this volume increase could play a crucial role in the formation of deep earthquakes as well as being of particular interest in materials science, in the study of energy-storing materials.

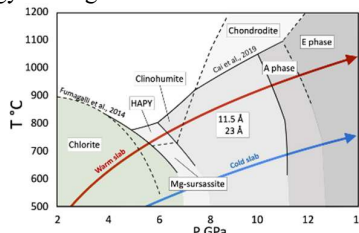


Figure 1. Water-bearing phases stability in the $\text{MgO-Al}_2\text{O}_3\text{-SiO}_2\text{-H}_2\text{O}$ system (modified after [3])

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