The real structure of tobermorite 11Å: normal and anomalous forms, OD character and polytypic modifications

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Abstract: Specimens of tobermorite 11Å from Wessels mine, South Africa, an ‘anomalous’ tobermorite, and from Bašcenov, Urals, Russia, a ‘normal’ tobermorite, have been studied through X-ray diffraction. Their structural disorder, evidenced by the diffuseness of the reflections with $k$ odd, has been dealt with through an OD approach, which allowed us to derive a reliable model of the structure, to define the two main polytypes (MDO structures), which were subsequently refined, revealing the distinctive structural details of the two specimens.

The MDO₁ polytype of tobermorite 11Å from Wessels mine [orthorhombic, space group $F2dd$, $a = 11.265(2)$, $b = 7.386(1)$, $c = 44.970(9)$ Å] was refined to $R = 0.128$, whereas the refinement carried on the MDO₂ polytype [monoclinic, space group $B11m$, $a = 6.735(2)$, $b = 7.385(1)$, $c = 22.487(4)$ Å, $\beta = 123.25(1)^\circ$] converged to $R = 0.051$. Two refinements were carried out for the MDO₂ polytype of the specimen from the Urals [space group $B11m$, $a = 6.732(2)$, $b = 7.368(1)$, $c = 22.680(4)$ Å, $\beta = 123.18(1)^\circ$] with data collected with conventional source ($R = 0.089$) and with synchrotron radiation ($R = 0.110$).

Common structural features are the infinite layers of calcium polyhedra, parallel to (001), with tetrahedral chains of wollastonite-type running along $b$ and attached on both sides of these layers. The composite layers are stacked along $c$ and connected through formation of double tetrahedral chains, with ‘ideal’ composition $[\text{Si}_6\text{O}_{15}(\text{OH})_2]$ and $[\text{Si}_6\text{O}_{16}(\text{OH})]$ in the specimens from Wessels mine and Urals respectively. The most distinctive feature of the two specimens is the content of the structural cavities: whereas only water molecules were found in the specimen from Wessels mine, ‘zeolitic’ calcium cations and water molecules were found in that from Urals. These structural aspects are compared and their relevance in explaining the different thermal behaviour of the two types of tobermorite 11Å is indicated.

Key-words: tobermorite 11Å, crystal structure, OD theory, double chains, thermal behaviour, normal tobermorite, anomalous tobermorite.

Introduction

Tobermorite was firstly described by Heddle (1880) from Tobermory (island of Mull in the Hebrides Archipelago) and from a quarry near Dunvegan in the island of Skye. Afterwards it was found in several other localities, generally in cavities of basic rocks or at the contact between limestone and dolerite, or granodiorites.

It was found that three distinct phases exist, corresponding to three degrees of hydration, tobermorite 9Å (riversideite), tobermorite 11Å (tobermorite s.s.), tobermorite 14Å (plombierite) (McConnell, 1954), characterised by different $d_{002}$ values in the powder diffraction pattern, 9.3 Å, 11.3 Å, 14.6 Å, from the least to the most hydrated form, respectively.

Most specimens are poorly crystalline or microcrystalline, not suitable for structural studies with single-crystal X-ray diffraction techniques. More-