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Tobermorites: Their real structure and order-disorder (OD) character

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ABSTRACT

The real structures of clinotobermorite, tobermorite 9 Å, and tobermorite 11 Å were determined through the application of OD approach, which allowed us to explain their peculiar disorder and polytypic features and to derive the main polytypes for each of them. The structural arrangements will be described and discussed for one polytype of each compound: clinotobermorite, triclinic polytype *C*1, $a = 11.274$, $b = 7.344$, $c = 11.468$ Å, $\alpha = 99.18°$, $\beta = 97.19°$, $\gamma = 90.03°$; tobermorite 9 Å, triclinic polytype $C\bar{1}$, $a = 11.156$, $b = 7.303$, $c = 9.566$ Å, $\alpha = 101.08°$, $\beta = 92.83°$, $\gamma = 89.98°$; tobermorite 11 Å, monoclinic polytype *B*11*m*, $a = 6.735$, $b = 7.385$, $c = 22.487$ Å, $\gamma = 123.25°$. Common structural features are infinite layers, parallel to (001), formed by sevenfold-coordinated calcium polyhedra. Tetrahedral double chains, built up through condensation of "Dreiereinfachketten" of wollastonite-type and running along **b**, link together adjacent calcium layers in clinotobermorite and tobermorite 11 Å, whereas single tetrahedral chains connect adjacent calcium layers in tobermorite 9 Å. The relatively wide channels of clinotobermorite and tobermorite 11 Å host "zeolitic" calcium cations and water molecules. The present structural results now allow for a sound discussion of the crystal chemical relationships between the various members of the tobermorite group and an explanation of the peculiar thermal behavior of tobermorite 11 Å.