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Pressure-induced phase transition in malayaite, $CaSnOSiO_4$

STEPHANIE RATH,[1,*] MARTIN KUNZ,[2] AND RONALD MILETICH[3]

[1]Labor für Kristallographie, ETH Zürich, Sonneggstrasse 5, CH-8092 Zürich, Switzerland
[2]Museum of Natural History, Augustinergasse 2, CH-4001 Basel, and Department of Earth Sciences, University of Basel, Bernoullistrasse 30, CH-4056 Basel, Switzerland
[3]Mineralogisches Institut, Universität Heidelberg, Im Neuenheimer Feld 236,D-69120 Heidelberg, Germany

ABSTRACT

A single crystal high-pressure diffraction study in a diamond-anvil cell shows that monoclinic malayaite ($CaSnOSiO_4$) transforms into a triclinic high-pressure polymorph at $P_c = 4.95(1)$ GPa. No discontinuity was observed for the individual crystallographic axes or the volume compressibility. Instead, the $A2/a - A\bar{1}$ phase transition reveals itself by significant deviations of the α and γ angles from 90°. The bulk elastic properties of the triclinic phase cannot be distinguished from those of the monoclinic structure within experimental uncertainty ($A2/a$: $V_0 = 389.68(3)$ Å^3, $K_0 = 121(1)$ GPa, and $K' = 4.2(5)$; $A\bar{1}$: $V_0 = 390.3(1)$ Å^3, $K_0 = 118.3(7)$ GPa, $K' = 4$). Fitting the compressibility to all data gives values of $V_0 = 389.64(3)$ Å^3, $K_0 = 121.6(7)$ GPa and $K' = 4.6(2)$. Structure refinements at four different pressures reveal the structural details of the monoclinic $A2/a$ and triclinic $A\bar{1}$ phases. Below the transition temperature the SiO_4 polyhedra show some non-rigid distortion, whereas the SnO_6 polyhedra remain almost unchanged. At the phase transition, the SiO_4 tetrahedra show further angular twisting while the SnO_6 chains shift parallel to $[\bar{1}01]$, inducing a reduction in symmetry. Furthermore, at pressures above 5 GPa the Ca atoms are displaced almost parallel to [100], causing a change in coordination from CaO_7 polyhedra to sheets of CaO_8 parallel to $(\bar{1}11)$.

At 7.394(4) GPa the cell parameters of the triclinic structure are $a = 6.9958(4)$ Å, $b = 8.8080(9)$ Å, $c = 6.4968(4)$ Å, $\alpha = 89.078(7)°$, $\beta = 112.745(5)°$, $\gamma = 91.230(7)°$, $V = 369.10(5)$ Å^3; space-group $A\bar{1}$.