*American Mineralogist, Volume 93, pages 53–62, 2008*

# Pressure-induced structural deformation and elastic behavior of wairakite

**Silvia Ori,[1] Simona Quartieri,[2,*] Giovanna Vezzalini,[1] and Vladimir Dmitriev[3]**

[1]Dipartimento di Scienze della Terra, Università di Modena e Reggio Emilia, via S. Eufemia 19, 41100 Modena, Italy
[2]Dipartimento di Scienze della Terra, Università di Messina, Salita Sperone 31, 98166 Messina S. Agata, Italy
[3]Swiss-Norwegian Beam Lines at ESRF, BP220, 38043 Grenoble Cedex, France

## Abstract

The elastic behavior and the high-pressure structural evolution of the zeolite wairakite [ideal chemical formula $Ca(Al_2Si_4O_{12})\cdot 2H_2O$, space group *I2/a*], the Ca-analog of analcime, have been investigated by means of in-situ synchrotron X-ray powder diffraction from ambient pressure to 7.8 GPa, and upon decompression. No complete X-ray amorphization is observed up to the highest investigated pressure, and the original unit-cell parameters are recovered upon decompression. The Rietveld structural refinements of the powder patterns converged successfully up to 2.5 GPa; above this pressure, a phase transition to triclinic symmetry is observed and only the unit-cell parameters were refined. An overall reduction of about 14% of the unit-cell volume between 0.0001 and 7.0 GPa is observed, demonstrating that wairakite is much more flexible upon compression than upon heating. The pressure dependence of the cell parameters is strongly anisotropic and larger after the transition to the triclinic space group. The elastic parameters refined with a second-order Birch-Murnaghan Equation of State are $V_0 = 2536(4)$ Å$^3$, $K_0 = 39(3)$ GPa, and $V_0 = 2632(38)$ Å$^3$, $K_0 = 24(3)$ GPa, for the monoclinic and triclinic phases, respectively.

The structure distortion of monoclinic wairakite, proceeding via tetrahedral tilting, induces deformations in the 4-, 6-, and 8-membered rings and an increase in the extra-framework Ca coordination number. A comparative discussion of the compressibility behavior of wairakite and analcime is reported.

**Keywords:** HP studies, XRD data, crystal structure, wairakite, phase transition, compressibility measurements