American Mineralogist, Volume 90, pages 28–35, 2005

The "template" effect of the extra-framework content on zeolite compression: The case of yugawaralite

ETTORE FOIS,[1] ALDO GAMBA,[1] GLORIA TABACCHI,[1] ROSSELLA ARLETTI,[2] SIMONA QUARTIERI,*[,3] AND GIOVANNA VEZZALINI[2]

[1]DSCA, Universita' dell'Insubria, via Lucini 3, I-22100 Como, Italy
[2]Dipartimento di Scienze della Terra, Largo S. Eufemia, 19, I-41100 Modena, Italy
[3]Dipartimento di Scienze della Terra, Salita Sperone 31, I-98166 Messina, S. Agata, Italy

ABSTRACT

The microscopic behavior of the Ca-zeolite yugawaralite has been studied by ab initio molecular dynamics simulations adopting experimental cell parameters obtained at pressures up to ~9 GPa. Pressure-induced volume contraction occurs via rotations of quasi-rigid TO_4 tetrahedra that reduce the size of the channels in which the extra-framework species are located. Such rotations are governed by deformation of the coordination polyhedron of Ca, which is made up of water and framework O atoms. Contraction of the Ca-H_2O distances is favored at moderate pressure; at higher pressure the shortening of Ca-framework O atom distances becomes prevalent. The hydrogen bond network plays a fundamental role in the overall response to pressure. Our results indicate that the high-*P*-induced deformation of the framework structure is strictly correlated to the extra-framework species that act as "templates" in the compression process.