ESRF	**Experiment title:** COMPRESSIBILITY BEHAVIOR OF ZEOLITES AND MIXED FRAMEWORK SILICATES WITH GIS AND GIS-RELATED STRUCTURES	**Experiment number**: 01-02-1005
Beamline: BM01a	**Date of experiment**: from: 09 giu 2013 to: 11 giu 2013	**Date of report**: 17/01/2015
Shifts: 12	**Local contact(s)**: Vladimir Dmitriev	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Rossella Arletti - Dipartimento di Scienze della Terra, Università di Torino, Italy

Simona Quartieri - Dipartimento di Fisica e Scienze della Terra, Università di Messina, Italy

Giovanna Vezzalini - Dipartimento di Scienze Chimiche e Geologiche, Università di Modena e Reggio Emilia, Italy

Lara Gigli - Dipartimento di Scienze della Terra, Università di Torino, Italy

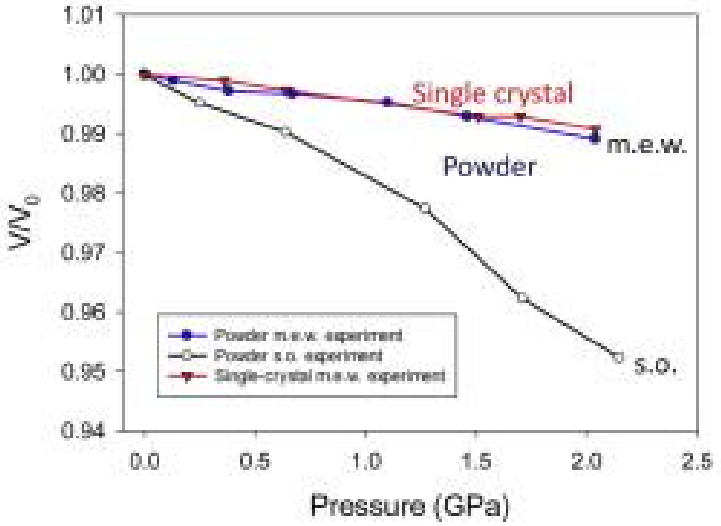
Danisi Rosa Micaela - Mineralogical Crystallography, Institute of Geological Sciences, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

Lara Leardini - Dipartimento di Fisica e Scienze della Terra, Università di Messina, Italy

Report:

The behavior of natural microporous cavansite and pentagonite, orthorhombic dimorphs of Ca(VO) (Si4O10)4H2O, was studied at high pressure by means of in situ synchrotron X-ray powder diffraction with a diamond anvil cell using two different pressure-transmitting fluids: methanol:ethanol: water = 16:3:1 (m.e.w.) and silicone oil (s.o.). In situ diffraction-data on a cavansite sample were collected up to 8.17(5) GPa in m.e.w, and up to 7.28(5) GPa in s.o. The high-pressure structure evolution was studied on the basis of structural refinements at 1.08(5), 3.27(5) and 6.45(5) GPa. The compressional behavior is strongly anisotropic. When the sample is compressed in s.o. from Pamb to 7.28(5) GPa, the volume contraction is 12.2%, whereas a, b and c decrease by 1.6%, 10.3% and 0.3%, respectively. The main deformation mechanisms at high-pressure are basically driven by variation of the Tï Oï T angles.
Powder diffraction data on a pentagonite sample were collected up to 8.26(5) GPa in m.e.w and 8.35(5) GPa in s.o. Additional single-crystal X-ray diffraction experiments were performed in m.e.w. up to 2.04(5) GPa. In both cases, pressure-induced over-hydration was observed in m.e.w. at high pressure. The penetration of a new H2O molecule leads to a stiffening effect of the whole structure. Moreover, between 2.45(5) and 2.96(5) GPa in m.e.w., a phase transition from an orthorhombic to a triclinic phase was observed. In s.o. pentagonite also transformed to a triclinic phase above 1.71(5) GPa. The overall compressibility of pentagonite and cavansite in s.o. is comparable, with a volume contraction of 11.6% and 12.2%, respectively.

STIFFENING OF PENTAGONITE STRUCTURE IN M.E.W.



Full details of the results in:

Danisi, R.M., Armbruster, T., Arletti, R., Gatta, G.D., Vezzalini., G., Quartieri, S., Dmitriev, V., (2015) Elastic behavior and pressure-induced structural modifications of the microporous $Ca(VO)Si_4O_{10}·4H_2O$ dimorphs cavansite and pentagonite, Microporous and mesoporous materials, 204, 257-268.