ESRF	**Experiment title:** Fluoride scheelites at high pressures: Li_2CaHfF_8	**Experiment number**: HS-2179
Beamline: BM01A	**Date of experiment**: from: 09/04/2004 to: 13/04/2004	**Date of report**: 10/09/2006
Shifts: 12	**Local contact(s)**: V. Dmitriev	*Received at ESRF:*

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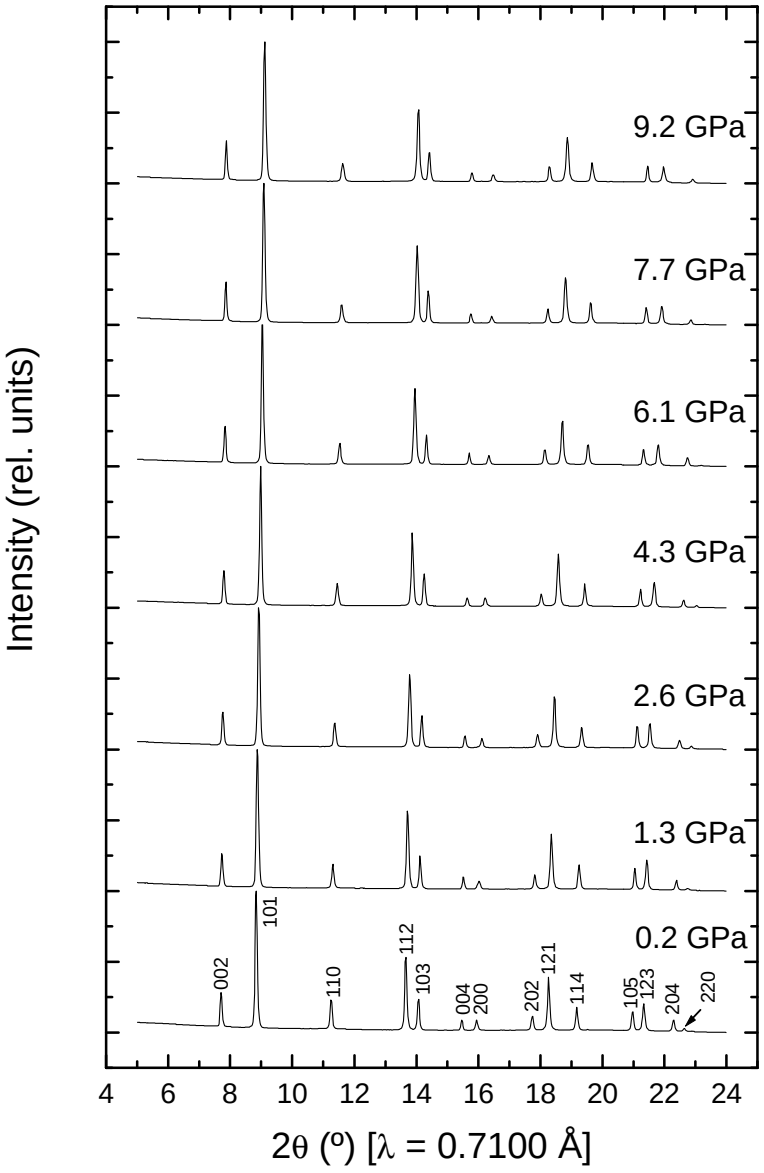
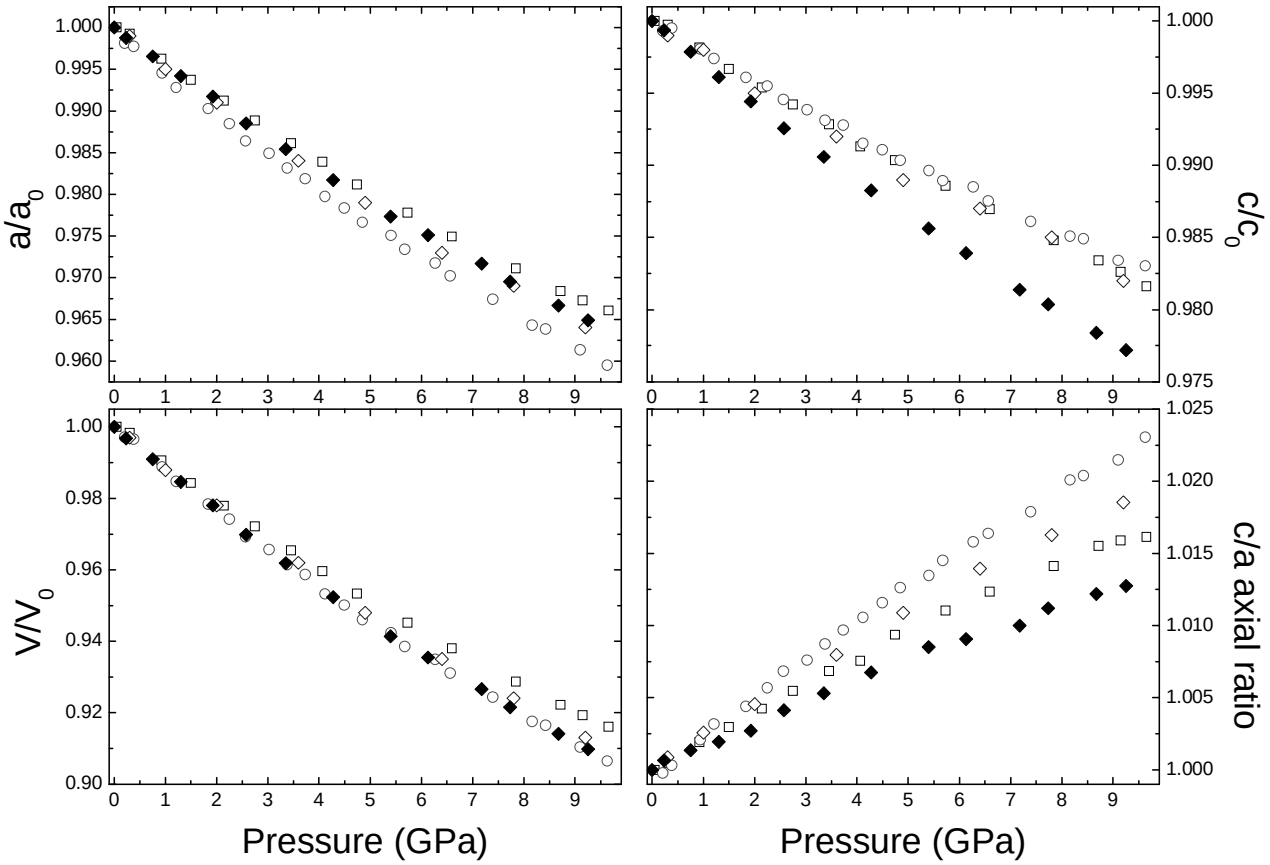
Report:

High-pressure behavior of Li_2CaHfF_8 scheelite ($I\bar{4}$, Z = 2) has been studied with synchrotron angle-dispersive powder and laboratory single-crystal x-ray diffraction using diamond anvil cells to 9.3 GPa at room temperature. The zero-pressure bulk modulus, its first pressure derivative, and the unit-cell volume at ambient pressure are B_0 = 78(3) GPa, B' = 4.42(64), and V_0 = 273.67(19) $Å^3$, respectively. The structural parameters obtained from the refinement of the single-crystal data show that all the polyhedra around the cations become more regular upon compression. The softest polyhedra are the CaF_8 units. Compared with previous investigations on $LiMF_4$ scheelites ($I4_1/1$, Z = 4; M: Y^{3+}, Gd^{3+}, or Lu^{3+}), our observations indicate that the compressibility mechanism in fluoride scheelites depends on the cationic substitution and distribution.



X-ray powder patterns of Li_2CaHfF_8 upon compression. Pressures are given in GPa. Miller indices mark the reflections of the scheelite.



Lattice parameters, unit-cell volumes, and c/a axial ratios for Li_2CaHfF_8 (full symbols), normalized to the respective values at atmospheric pressure. They are compared with the high-pressure data for $LiYF_4$ (open blue symbols), $LiGdF_4$ (open red symbols), and $LiLuF_4$ (open black symbols).