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Structural transitions and electron transfer in coffinite, $USiO_4$, at high pressure

F.X. Zhang,[1] V. Pointeau,[1] L.C. Shuller,[1] D.M. Reaman,[2] M. Lang,[1] Zhenxian Liu,[3] Jingzhu Hu,[4] W.R. Panero,[2] U. Becker,[1] C. Poinssot,[5] and R.C. Ewing[1,*]

[1]Department of Geological Sciences, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.
[2]School of Earth Sciences, Ohio State University, Columbus, Ohio 43210, U.S.A.
[3]Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C. 20015, U.S.A.
[4]Mineral Physics Institute and Department of Geosciences, Stony Brook University, Stony Brook, New York 11794, U.S.A.
[5]Nuclear Energy Division, Department of Radiochemistry and Processes, Commissariat à l'Energie Atomique—CEA Marcoule, 30200 Bagnols-Sur-Cèze Cedex, France

Abstract

The compressibility, phase stability, and vibrational properties of coffinite ($USiO_4$) were studied by in situ X-ray diffraction and infrared (IR) measurements at high pressures. An irreversible phase transition from the zircon-type to scheelite-type structure was found to occur at 14–17 GPa. Accompanying the structural transition, partial amorphization was also evident in the XRD analysis. The predicted transition pressure calculated by density functional theory is in good agreement with the experimental results. IR spectra also suggest that water is incorporated into the coffinite structure, and a pressure-induced electron transfer ($U^{4+} \rightarrow U^{5+}$) may also occur.

Keywords: Coffinite, high pressure, phase transition, XRD, IR