In Situ Raman Spectroscopy of Uranyl Peroxide Nanoscale Cage Clusters Under Hydrothermal Conditions

Haylie L. Lobeck,^a Hrafn Traustason,^b Patrick A. Julien,^c John R. FitzPatrick,^a Sara Mana,^d Jennifer E. S. Szymanowski,^a and Peter C. Burns * ^{a, b}

^a Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN 46556, USA

^b Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, USA

^c Department of Chemistry, McGill University, Montreal, Quebec, Canada H3A 0B8

^d Department of Geological Sciences, Salem State University, Salem, MA 01970, USA

*To whom correspondence should be addressed. Email: pburns@nd.edu

Electronic Supplementary Information



Fig. S1 PXRD pattern of synthetic compreignacite compared to ICDD database PDF # 00-033-1049 K₂[(UO₂)₆O₄(OH)₆(H₂O)₈.



Fig. S2 Custom made sapphire tube and Teflon stopper with wire closure created by Rayotek Scientific, Inc.



Fig. S3 Measured thermograph of the heating cycle used for *in situ* Raman experiments.



Fig. S4 Observed Raman shifting of the most intense sapphire peak verses temperature.



Fig. S5 PXRD Patterns of solids resulting from heating U_{60} solutions between 120°C and 180°C.



Fig. S6 SEM images of solids resulting from heating U_{60} solutions between 120°C and 180°C.



Fig. S7 SEM images of solids resulting from heating $U_{60}Ox_{30}$ solutions between 130°C and 180°C.