Supplementary Information for: Multimodal X-ray microanalysis of a UFeO₄:

evidence for the environmental stability of ternary U(V) oxides from depleted uranium munitions testing

Daniel E. Crean¹, Martin C. Stennett¹, Francis R. Livens², Daniel Grolimund³, Camelia N. Borca³ and Neil C. Hyatt¹*

1 – Immobilisation Science Laboratory, Department of Materials Science and Engineering, The University of Sheffield, UK
2 – Centre for Radiochemistry Research, Department of Chemistry, The University of Manchester, UK
3 – Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Figure S1: Calibration relationship used for determination of oxidation state. UYT is U₀.₅Y₀.₅Ti₂O₆

Figure S2: XANES data showing selection of excitation energies for chemical speciation imaging and calibration relationships used for determination of oxidation state. UYT is U₀.₅Y₀.₅Ti₂O₆

*Corresponding author: n.c.hyatt@sheffield.ac.uk
Figure S3: Comparison of computed $k^2 \chi(k)$ and $|\text{FT } k^2 \chi(k)|$ for plausible bounding contributions of U(IV) and U(VI) environments to average a U(V) environment in UFeO$_4$, assuming charge compensation by Fe(III) and/or Fe(II). Both uranyl and non-uranyl U(VI) environments are considered. See text for details of calculations.