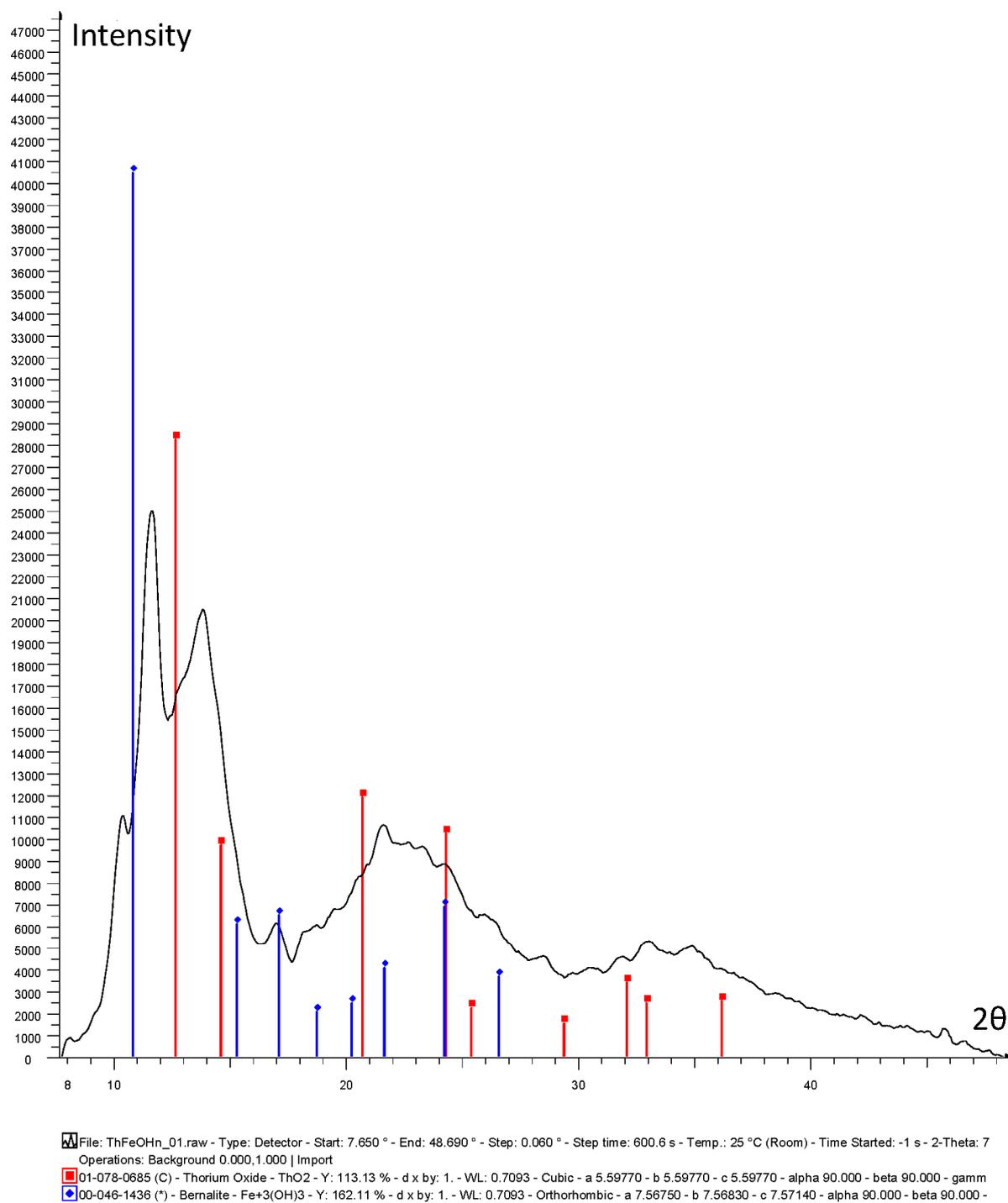


## Formation of a heteronuclear hydrolysis complex in the Th<sup>IV</sup>/Fe<sup>III</sup> system

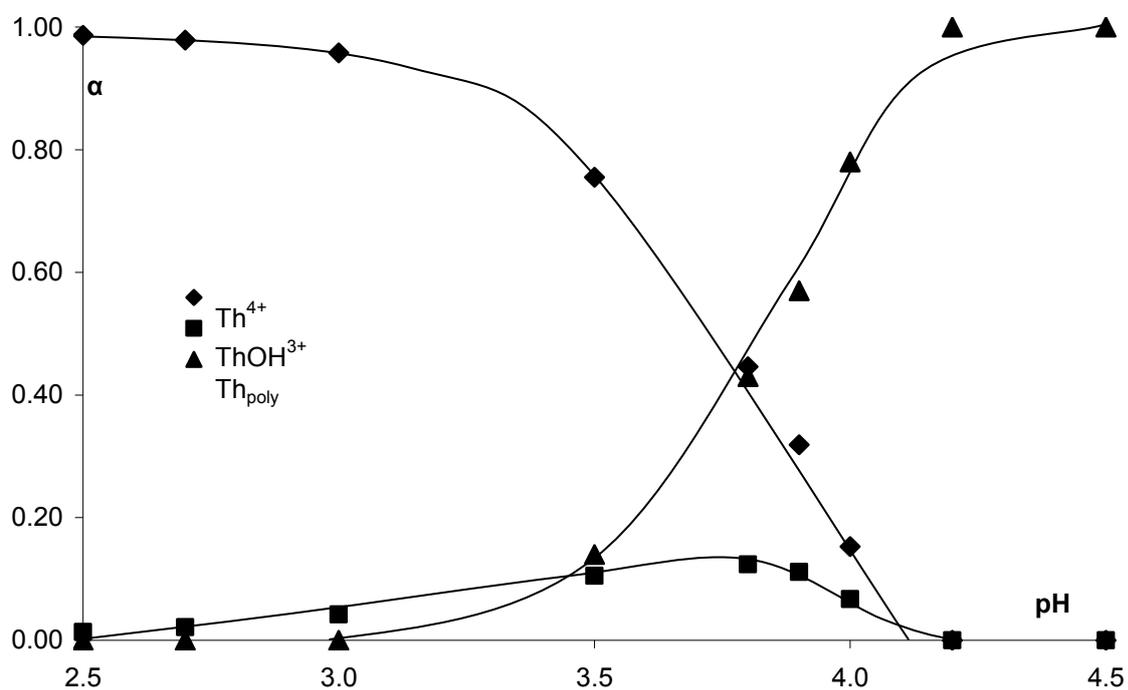
Natallia Torapava,<sup>a</sup> Artsiom Radkevich,<sup>b</sup> Ingmar Persson,<sup>a\*</sup> Dmitri Davydov<sup>b</sup> and Lars Eriksson<sup>c</sup>

### **Electronic Supplementary Information**

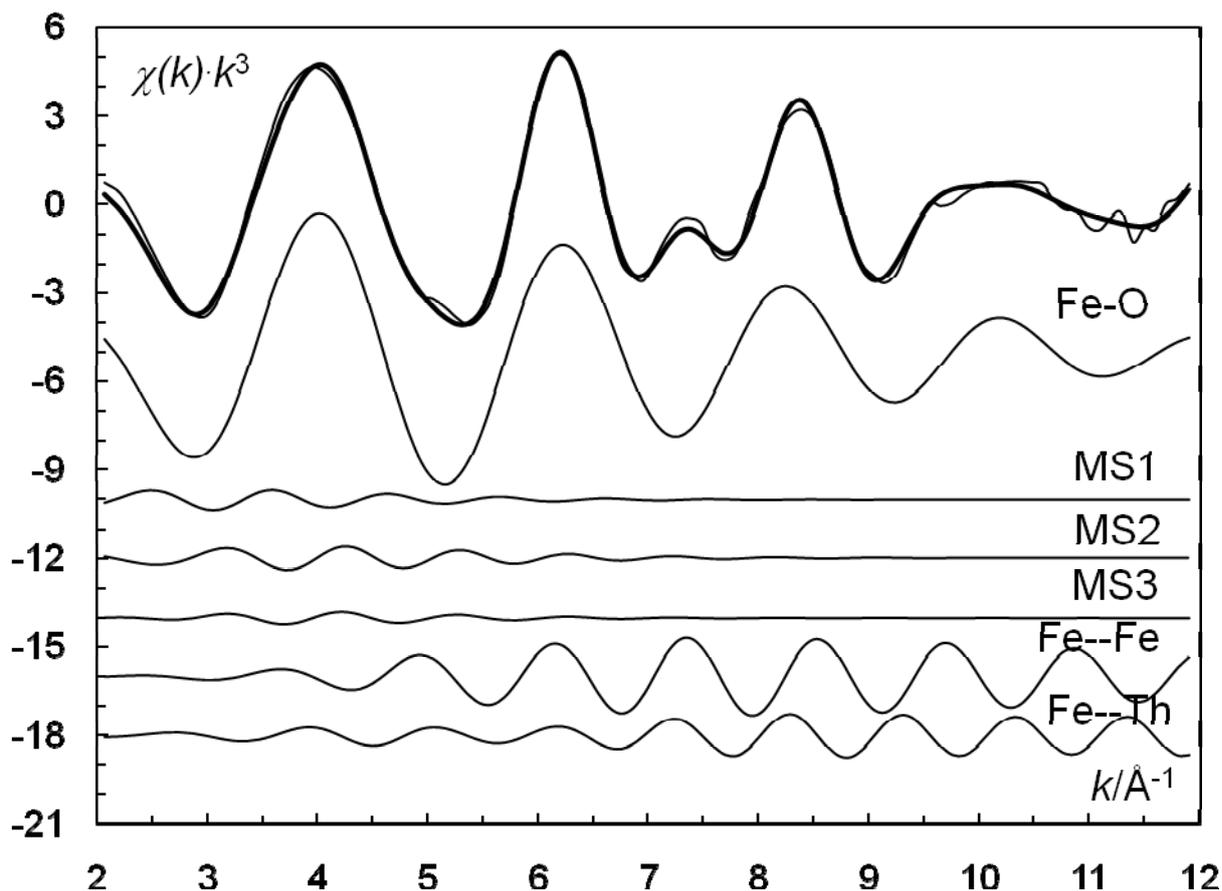
**Figure S1.** XRD patterns for A-3.5 after increasing pH to about 12.



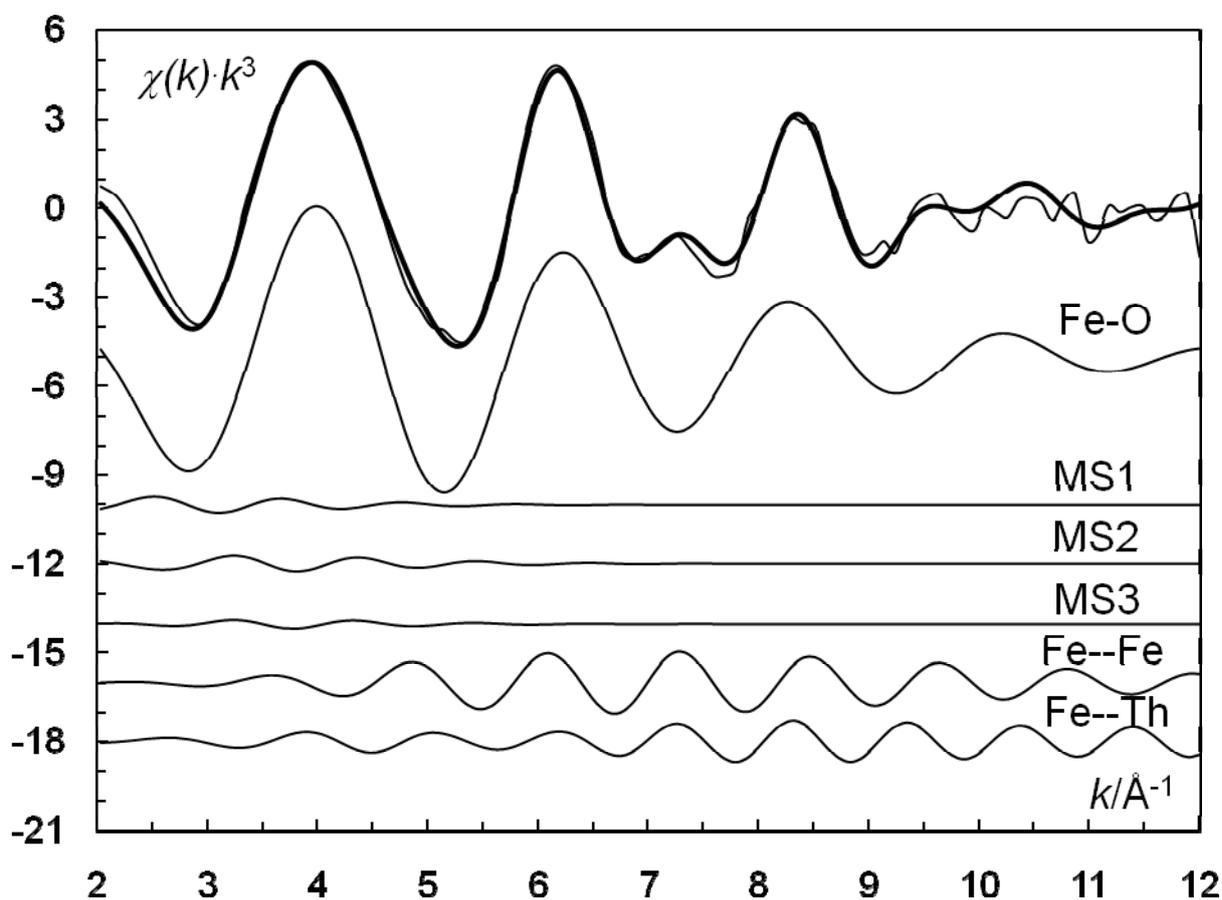
**Figure S2.** Diagram of thorium(IV) species distribution at  $C_{\text{Th}} = 1 \cdot 10^{-2} \text{ mol} \cdot \text{cm}^{-3}$  at different pH values ( $\alpha$  – part of thorium(IV) present as polynuclear species) .



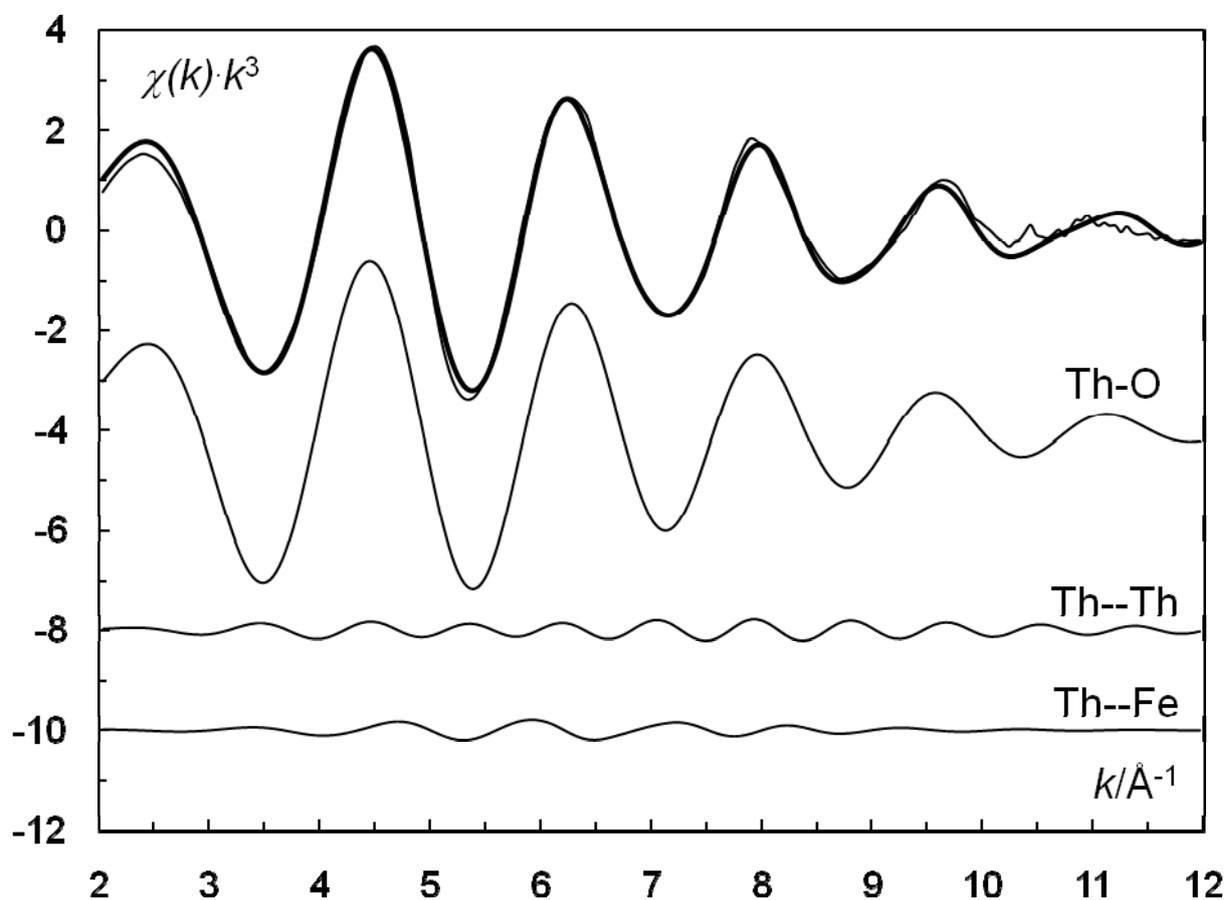
**Figure S3a.** Fit and the individual contribution of the different scattering paths of the Fe K edge EXAFS data of solution A-2.9, thin line – experimental data, thick line - calculated model function using the parameters given in Table 2, and the individual contributions of single scattering Fe-O (offset -6), multiple scattering within FeO<sub>6</sub> (offsets -10, -12 and -14), single scattering Fe···Fe (offset -16), and single scattering Fe···Th (offset -18).



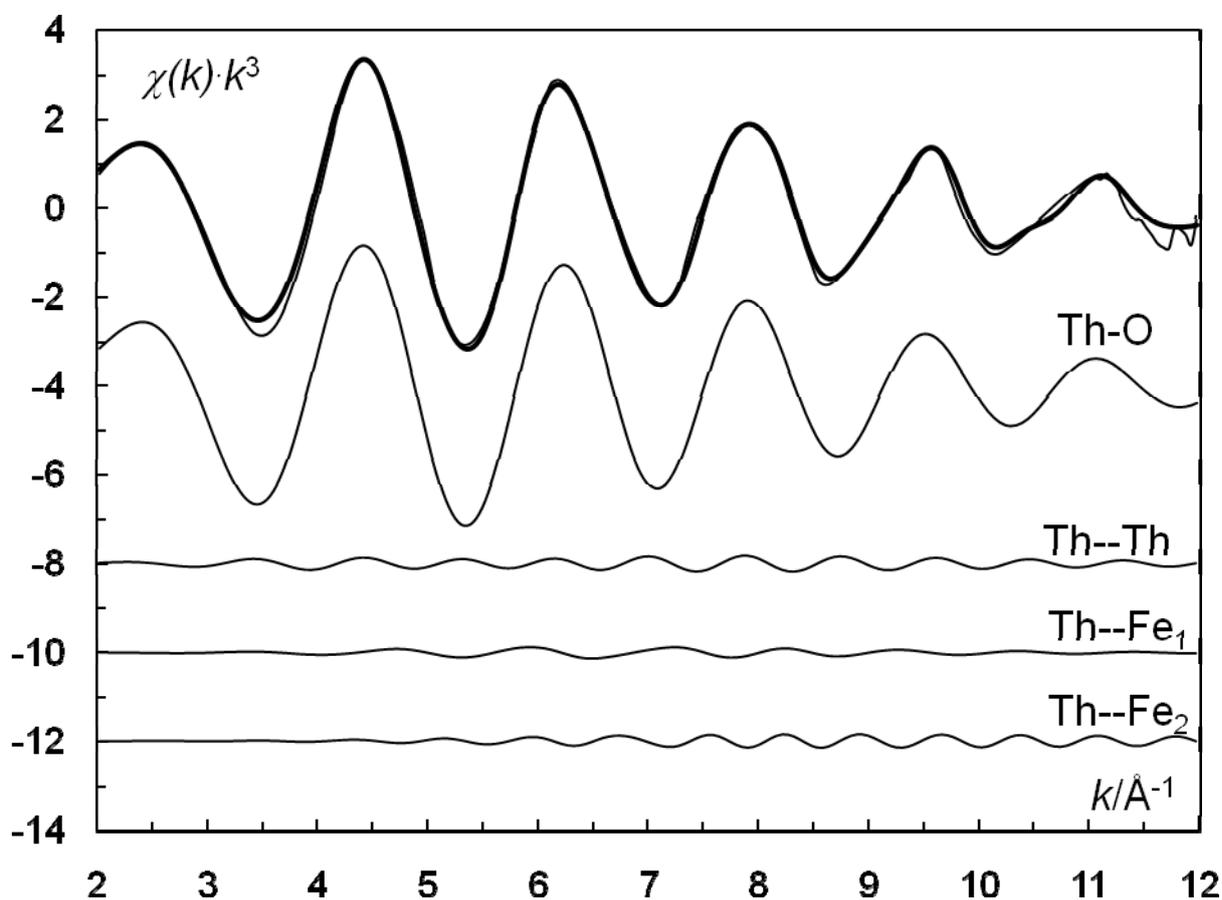
**Figure S3b.** Fit and the individual contribution of the different scattering paths of the Fe K edge EXAFS data of solution C-2.9, thin line – experimental data, thick line - calculated model function using the parameters given in Table 2, and the individual contributions of single scattering Fe-O (offset -6), multiple scattering within FeO<sub>6</sub> (offsets -10, -12 and -14), single scattering Fe···Fe (offset -16), and single scattering Fe···Th (offset -18).



**Figure S3c.** Fit and the individual contribution of the different scattering paths of the Th  $L_3$  edge EXAFS data of solution A-2.9, thin line – experimental data, thick line - calculated model function using the parameters given in Table 2, and the individual contributions of single scattering Th-O (offset -4), single scattering Th··Th (offset -8) and single scattering Th··Fe (offset -10).



**Figure S3d.** Fit and the individual contribution of the different scattering paths of the Th  $L_3$  edge EXAFS data of solution C-2.9, thin line – experimental data, thick line - calculated model function using the parameters given in Table 2, and the individual contributions of single scattering Th-O (offset -4), single scattering Th··Th (offset -8), single scattering Th··Fe<sub>1</sub> (offset -10), and single scattering Th··Fe<sub>2</sub> (offset -12).



**Figure S4.** UV-visible spectra of Th<sup>IV</sup>/Fe<sup>III</sup> solutions, series A.

