Supplementary Materials

A Combined Extended X-ray Absorption Fine Structure Spectroscopy and Density Functional Theory Study of Americium vs. Yttrium Adsorption on Corundum (α–Al_2O_3)

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Table S1. Sample description and results obtained from **A)** isotherm experiment 1, containing Eu^{3+} only, **B)** isotherm experiment 2, containing varying concentrations of Eu^{3+} and a constant Y^{3+} concentration of 10^{-6} mol/L and **C)** isotherm experiment 3, containing varying concentrations of Eu^{3+} and a constant Y^{3+} concentration of 10^{-4} mol/L. Buffered samples containing 0.01 mol/L TRIS buffer (tris(hydroxymethyl) aminomethane) in 0.01 mol/L $NaClO_4$ were used to avoid pH fluctuations. A constant concentration of 1.3×10^{-9} mol/L radioactive ^{152}Eu was added to all samples, and the overall Eu^{3+} concentration was adjusted with of a commercial 1,000 ppm Eu^{3+} standard solution in 0.5 mol/L HNO_3. In the isotherms with Y^{3+} as competing metal, Y^{3+} was added to the samples from a commercial 1,000 ppm Y^{3+} standard in 0.5 mol/L HNO_3. The addition of the trivalent metal cations was done simultaneously to the corundum containing suspensions. Sample pH adjustment was carried out over several days to avoid precipitation of Eu:$Y(OH)_3$ from oversaturated solutions. After an equilibrium time of one week, the solution was separated from the solid phase via centrifugation. The ^{152}Eu concentration was measured with liquid scintillation counting. The precision of the pH–measurements is ± 0.1.

A) Isotherm experiment 1							
Sample No.	pH_{eq}	$c(Eu^{3+})$, initial (mol/L)	$c(Y^{3+})$, initial (mol/L)	$c(\alpha\text{-}Al_2O_3)$ (g/L)	Eu^{3+} adsorbed (%)	Eu^{3+} adsorbed (mol/kg)	Eu^{3+} in solution (mol/L)
1	8.27	1.30×10^{-9}			99.97	2.60×10^{-6}	4.17×10^{-13}
2	8.24	6.30×10^{-9}			99.96	1.26×10^{-5}	2.85×10^{-12}
3	8.23	8.80×10^{-9}			99.96	1.76×10^{-5}	3.66×10^{-12}
4	8.25	1.13×10^{-8}			99.96	2.26×10^{-5}	4.70×10^{-12}
5	8.25	2.63×10^{-8}			99.99	5.26×10^{-5}	2.78×10^{-12}
6	8.25	7.63×10^{-8}			99.95	1.53×10^{-4}	4.18×10^{-11}
7	8.16	7.51×10^{-7}			99.98	1.50×10^{-3}	1.33×10^{-10}
8	8.22	1.00×10^{-6}	0	0.5	99.96	2.00×10^{-3}	4.53×10^{-10}
9	8.24	$2.50E\times10^{-6}$			99.95	5.00×10^{-3}	1.19×10^{-9}
10	8.25	5.00×10^{-6}			99.98	1.00×10^{-2}	8.27×10^{-10}
11	8.25	7.50×10^{-6}			99.79	1.50×10^{-2}	1.57×10^{-9}
12	8.25	1.00×10^{-5}			99.35	1.99×10^{-2}	6.52×10^{-8}
13	8.24	2.50×10^{-5}			97.83	4.89×10^{-2}	5.42×10^{-7}
14	8.25	5.00×10^{-5}			93.87	9.39×10^{-2}	3.07×10^{-6}
15	8.27	7.50×10^{-5}			87.71	1.32×10^{-2}	9.22×10^{-6}

16	8.27	1.00×10^{-4}			89.67	1.79×10^{-2}	1.03×10^{-5}

B) Isotherm experiment 2

Sample No.	pH_{eq}	$c(Eu^{3+})$, initial (mol/L)	$c(Y^{3+})$, initial (mol/L)	$c(\alpha\text{-}Al_2O_3)$ (g/L)	Eu^{3+} adsorbed (%)	Eu^{3+} adsorbed (mol/kg)	Eu^{3+} in solution (mol/L)
1	8.33	1.3×10^{-9}			99.06	2.58×10^{-6}	1.22×10^{-11}
2	8.34	6.30×10^{-9}			99.08	1.25×10^{-5}	5.77×10^{-11}
3	8.35	8.80×10^{-9}			99.01	1.74×10^{-5}	8.70×10^{-11}
4	8.35	1.13×10^{-8}			99.06	2.24×10^{-5}	1.06×10^{-10}
5	8.35	2.63×10^{-8}			99.12	5.21×10^{-5}	2.31×10^{-10}
6	8.36	5.13×10^{-8}			99.15	1.02×10^{-4}	4.37×10^{-10}
7	8.36	7.63×10^{-8}			99.21	1.51×10^{-4}	6.06×10^{-10}
8	8.35	1.01×10^{-7}			98.89	2.00×10^{-4}	1.12×10^{-9}
9	8.35	2.51×10^{-7}	10^{-6}	0.5	96.42	4.85×10^{-4}	9.01×10^{-9}
10	8.36	5.01×10^{-7}			99.00	9.93×10^{-4}	5.03×10^{-9}
11	8.33	7.51×10^{-7}			99.21	1.49×10^{-3}	5.97×10^{-9}
12	8.33	1.00×10^{-6}			98.76	1.98×10^{-3}	1.25×10^{-9}
13	8.33	2.50×10^{-6}			98.87	4.95×10^{-3}	2.82×10^{-8}
14	8.35	5.00×10^{-6}			98.17	9.82×10^{-3}	9.16×10^{-8}
15	8.36	7.50×10^{-6}			97.61	1.46×10^{-2}	1.79×10^{-7}
16	8.34	1.00×10^{-5}			96.57	1.93×10^{-2}	3.43×10^{-7}
17	8.34	2.50×10^{-5}			95.38	4.77×10^{-2}	1.16×10^{-6}
18	8.34	5.00×10^{-5}			93.88	9.39×10^{-2}	3.06×10^{-6}

C) Isotherm experiment 3

Sample No.	pH_{eq}	$c(Eu^{3+})$, initial (mol/L)	$c(Y^{3+})$, initial (mol/L)	$c(\alpha\text{-}Al_2O_3)$ (g/L)	Eu^{3+} adsorbed (%)	Eu^{3+} adsorbed (mol/kg)	Eu^{3+} in solution (mol/L)
1	8.31	1.3×10^{-9}			89.78	2.33×10^{-6}	1.33×10^{-10}
2	8.31	6.30×10^{-9}			90.56	1.14×10^{-5}	5.95×10^{-10}
3	8.26	8.80×10^{-9}			86.84	1.53×10^{-5}	1.16×10^{-9}
4	8.28	1.13×10^{-8}			87.94	1.99×10^{-5}	1.36×10^{-9}
5	8.26	2.63×10^{-8}			90.11	4.74×10^{-5}	2.60×10^{-9}
6	8.25	5.13×10^{-8}			74.53	7.65×10^{-5}	1.31×10^{-8}
7	8.25	7.63×10^{-8}			88.02	1.34×10^{-4}	9.14×10^{-9}
8	8.26	1.01×10^{-7}	10^{-4}	0.5	89.21	1.81×10^{-4}	1.09×10^{-8}
9	8.23	2.51×10^{-7}			87.02	4.37×10^{-4}	3.26×10^{-8}
10	8.25	5.01×10^{-7}			88.24	8.85×10^{-4}	5.90×10^{-8}
11	8.19	7.51×10^{-7}			88.07	1.32×10^{-3}	8.96×10^{-8}
12	8.24	1.00×10^{-6}			88.33	1.77×10^{-3}	1.17×10^{-7}
13	8.22	2.50×10^{-6}			87.75	4.39×10^{-3}	3.07×10^{-7}
14	8.23	5.00×10^{-6}			82.06	8.21×10^{-3}	8.97×10^{-7}
15	8.26	7.50×10^{-6}			77.24	1.16×10^{-2}	1.71×10^{-6}

16	8.26	1.00×10^{-5}		79.98	1.60×10^{-2}	2.00×10^{-6}
17	8.27	2.50×10^{-5}		77.58	3.88×10^{-2}	5.61×10^{-6}

Table S2. Summary of EXAFS sample parameters. The background electrolyte in the experiments was 0.01 mol/L $NaClO_4$. The ^{243}Am stock solution concentration was 5.96 $\times 10^{-2}$ mol/L in 1 mol/L HCl. Yttrium was applied from a 0.2 mol/L Y^{3+} stock solution prepared by dissolving $YCl_3 \times 6H_2O$ in 0.01 mol/L $HClO_4$. Sample pH adjustment was carried out over several days to avoid precipitation of $Am:Y(OH)_3$ from oversaturated solutions. An equilibrium time of two days after the last pH adjustment was used before phase separation. The ^{243}Am concentration was measured with γ–counting. The precision of the pH–measurements is ± 0.1.

Sample	pH_{eq}	$c(Am^{3+})$, initial (mol/L)	$c(Y^{3+})$, initial (mol/L)	$c(\alpha\text{-}Al_2O_3)$ (g/L)	Am^{3+} adsorbed (%)	Am^{3+} adsorbed (mol/kg)	Am^{3+} in solution (mol/L)
1	8.41	6×10^{-6}	0	2	99.99	3.00×10^{-3}	6.00×10^{-10}
2	8.46	2×10^{-5}	0	2	99.98	1.00×10^{-2}	4.00×10^{-9}
3	8.47	6×10^{-6}	2×10^{-5}	2	99.60	2.99×10^{-3}	2.40×10^{-8}
4	8.48	2×10^{-5}	2×10^{-5}	2	99.34	9.93×10^{-3}	1.32×10^{-7}
5	8.50	2×10^{-5}	2×10^{-4}	2	96.91	9.73×10^{-3}	5.34×10^{-7}