

**Supporting Information of :**  
**Hydration properties and ionic radii of actinide(III) ions in aqueous solution**

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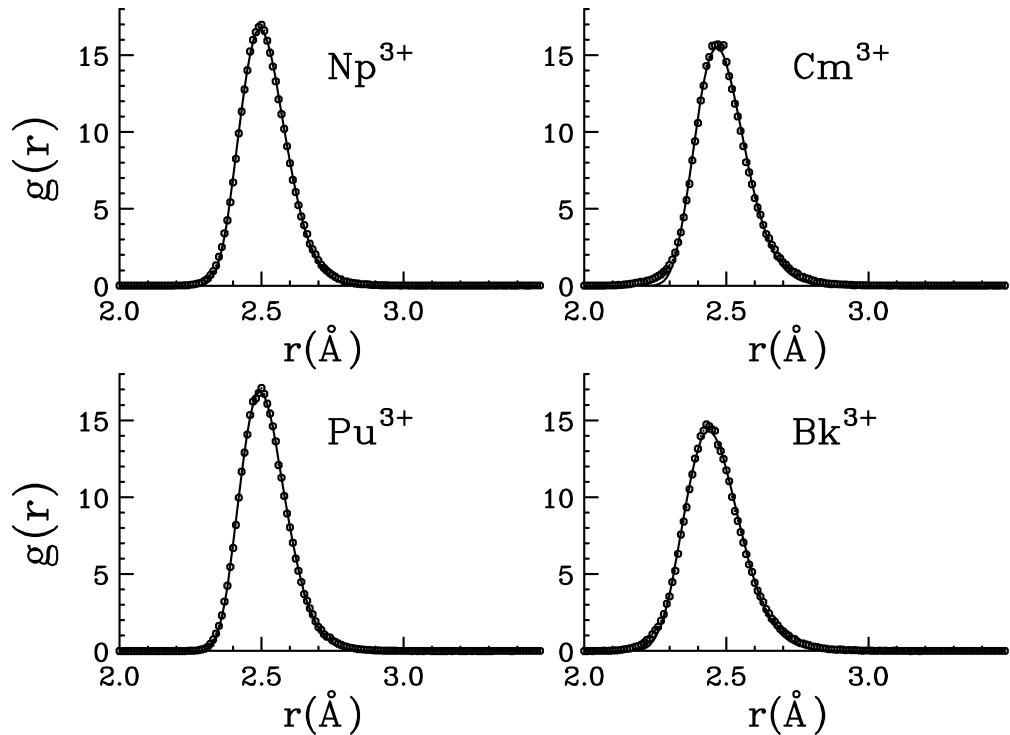
**Table S1.** Parameters of the An(III)-water force field employed in the DM simulations.

	$B_{An-O}$ [ $\text{\AA}^{-1}$ ]	$C_{An-O}/10^{+4}$ [ $\text{kJ mol}^{-1} \text{\AA}^6$ ]	$\alpha$ [ $\text{\AA}^3$ ]
U(III)	3.483	3.7464	1.846
Np(III)	3.500	3.6384	1.633
Pu(III)	3.517	3.5342	1.486
Am(III)	3.534	3.4334	1.363
Cm(III)	3.551	3.3359	1.238
Bk(III)	3.596	3.0953	1.197
Cf(III)	3.613	3.0086	1.166

**Table S2.** An-O first shell structural parameters of An(III) ions in aqueous solution obtained from the MD simulations. N is the coordination number, R is the average distance,  $\sigma^2$  is the Debye-Waller factor, and  $\beta$  is the asymmetry parameter.

	N	R [ $\text{\AA}$ ]	$\sigma^2$ [ $\text{\AA}^2$ ]	$\beta$
U-O	9.0	2.54	0.010	0.40
Np-O	9.0	2.52	0.007	0.42
Pu-O	9.0	2.51	0.007	0.44
Am-O	9.0	2.49	0.007	0.49
Cm-O	8.9	2.48	0.008	0.47
Bk-O	8.9	2.45	0.009	0.46
Cf-O	8.9	2.43	0.009	0.45

**Figure S1.** An-O  $g(r)$ 's obtained from MD simulations of An(III) ions in aqueous solution (dotted line) and corresponding gamma-like asymmetric peaks obtained from the fitting procedure (solid line).



**Figure S2.** Upper panels: fits of the L<sub>3</sub>-edge EXAFS spectra of An(III) ions in aqueous solution (red dotted line is experimental data, blue full line is theoretical model) by using a two-shell model. Lower panels: nonphase-shift-corrected Fourier transform of the experimental data (red dotted line) and of the total theoretical signal (blue full line).

