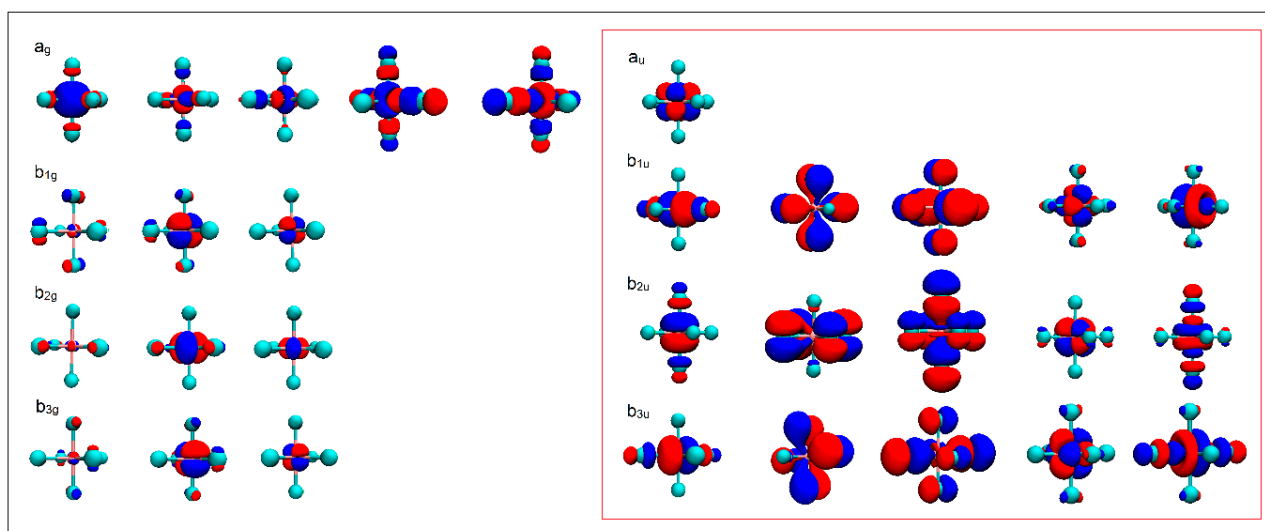


# Supplementary Materials

**Table S1.** Gas-phase (GP) and aqueous-phase (AP) calculated optimal bond-lengths for all complexes considered in this study.

Complex	State	$r_{M-Cl}$ (Å)					
		RASPT2		B3LYP		PBE	
		GP	AP	GP	AP	GP	AP
[U(VI)Cl <sub>6</sub> ]	<sup>1</sup> A <sub>g</sub>	2.51	2.48	2.49	2.47	2.48	2.48
[U(V)Cl <sub>6</sub> ] <sup>-</sup>	<sup>2</sup> A <sub>u</sub>	2.56	2.54	2.56	2.55	2.56	2.55
[U(IV)Cl <sub>6</sub> ] <sup>2-</sup>	<sup>3</sup> B <sub>1g</sub> / <sup>3</sup> B <sub>2g</sub> / <sup>3</sup> B <sub>3g</sub>	2.71	2.69	2.69	2.66	2.69	2.65
[U(III)Cl <sub>6</sub> ] <sup>3-</sup>	<sup>4</sup> A <sub>u</sub>	2.90	2.89	2.90	2.83	2.90	2.80
[Ce(IV)Cl <sub>6</sub> ] <sup>2-</sup>	<sup>1</sup> A <sub>g</sub>	2.68	2.64	2.67	2.66	2.67	2.65
[Ce(III)Cl <sub>6</sub> ] <sup>3-</sup>	<sup>2</sup> B <sub>1u</sub> / <sup>2</sup> B <sub>2u</sub> / <sup>2</sup> B <sub>3u</sub>	2.93	2.86	2.88	2.82	2.86	2.79



**Figure S1.** Orbitals included in the RAS (black box) and CAS calculations (red box).