Supporting Information for: *Speciation of Curium(III) Ion in Aqueous Solution: A Combined Study by Quantum Chemistry and Molecular Dynamics Simulation* by Tianxiao Yang and Bruce E. Bursten

Figure S1. Optimized structure of $[\text{Cm}(\text{H}_2\text{O})_6(\text{H}_2\text{O})_1]^{3+}$ in $C_1$ point group symmetry at the B3LYP/6-311G* level in aqueous phase.
Figure S2. Optimized structure of (a) \([\text{Cm(H}_2\text{O)}_{10}]^{3+}\) of \(D_2\) point group symmetry, (b) \([\text{Cm(H}_2\text{O)}_{10}]^{3+}\) of \(D_{5d}\) point group symmetry, (c) \([\text{Cm(H}_2\text{O)}_8\text{(H}_2\text{O)}_2]^{3+}\) of \(C_1\) point group symmetry and (d) \([\text{Cm(H}_2\text{O)}_9\text{(H}_2\text{O)}_1]^{3+}\) of \(C_s\) point group symmetry at the B3LYP/6-311G* level in aqueous phase.
Figure S3. Optimized structure of (a) $[\text{Cm(H}_2\text{O})_8\text{(H}_2\text{O})_4]^{3+}$ in $D_2$ point group symmetry, (b) $[\text{Cm(H}_2\text{O})_9\text{(H}_2\text{O})_3]^{3+}$ in $C_1$ point group symmetry and (c) $[\text{Cm(H}_2\text{O})_{10}\text{(H}_2\text{O})_2]^{3+}$ in $C_1$ point group symmetry at the B3LYP/6-311G* level in aqueous phase.
Figure S4. Optimized structure of $[\text{Cm(H}_2\text{O)}_{18}\text{(H}_2\text{O)}_{15}\text{(H}_2\text{O)}_3]^ {3+}$. 

7.25 Å
Figure S5. Residence probability $p(t)$ that a water molecule still belongs to the second hydration shell after a correlation time $t$ calculated from MD simulation. Exponential fits are shown as solid line.
Figure S6. Curium-oxygen distance for a 70 ps interval. The water exchange events between the second hydration shell and the bulk were observed.