Electronic supplementary information for:

Displacement of carbonates from $Ca_2UO_2(CO_3)_3$ by amidoxime-based ligands from free-energy simulations

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1. Force field parameters of $Ca_2UO_2(CO_3)_3$ used in this work:

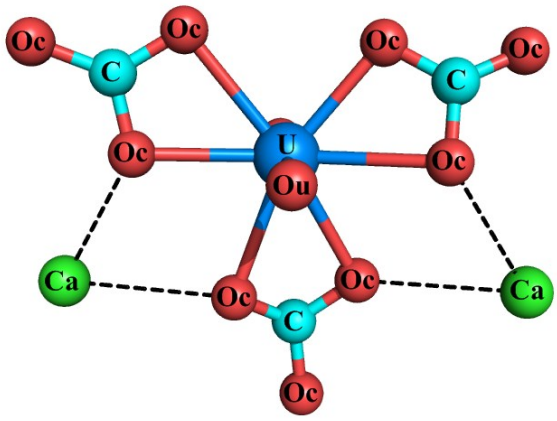

Fig. S1. Atom labels in the $Ca_2UO_2(CO_3)_3$ complex for Table S1-S6.

Table S1. Elemental symbols and charges.

Species	*Charge (|e|)*	Species	*Charge (|e|)*
Uranium (U)	+2.5	Water Oxygen (Ow)	-0.8340
Uranium Oxygen (Ou)	-0.25	Water hydrogen (Hw)	+0.4170
Calcium (Ca)	+2.0000	Carbon (C)	+1.135
Sodium (Na)	+1.0000	Carbonate Oxygen (Oc)	-1.045
Chloride (Cl)	-1.0000		

Table S2. Bond stretching: $V(r) = K(r_{ij} - r_0)^2$

Species	K (kcal·mol^{-1}·Å^{-2})	r_0 (Å)
U-Ou	500.00	1.80
C-Oc	1568.45	1.18
Ow-Hw	553.0	0.9572
Hw-Hw	553.0	1.5136

Table S3. Bond bending: $V(\theta) = K(\theta_{ijk} - \theta_0)^2$

Species	K (kcal·mol^{-1}·rad^{-2})	θ_0 (deg)
Ou-U-Ou	150.000	180
Oc-C-Oc	320	120

Table S4. Improper torsion potential parameters within a carbonate group and the carbonate-U complex: $V(\varphi) = K[1 + cos(2\varphi_{ijkl} - \varphi_0)]$

Species	K (kcal·mol^{-1})	φ_0 (deg)	n
Oc-Oc-C-Oc	2.6	180	2

Table S5. Lennard-Jones potential parameters: $V(r) = \varepsilon[(R^*/r)^{12} - 2(R^*/r)^6]$

Ion	ε (kcal·mol^{-1})	R^* (Å)
U–U	0.1200	1.6000
Ou–Ou	0.200	1.7500
Oc–Oc	0.1554	1.7766
C–C	0.0860	1.9080
Ca^{2+}– Ca^{2+}	0.4598	1.7131
Na^+–Na^+	0.0874393	1.369
Cl^-–Cl^-	0.0355910	2.513
Ow–Ow	0.1520	1.7683
Hw–Hw	--	--
U–Oc	0.111613	1.812889

2. Free-energy profiles for the association of CO_3^{2-} with Ca^{2+}

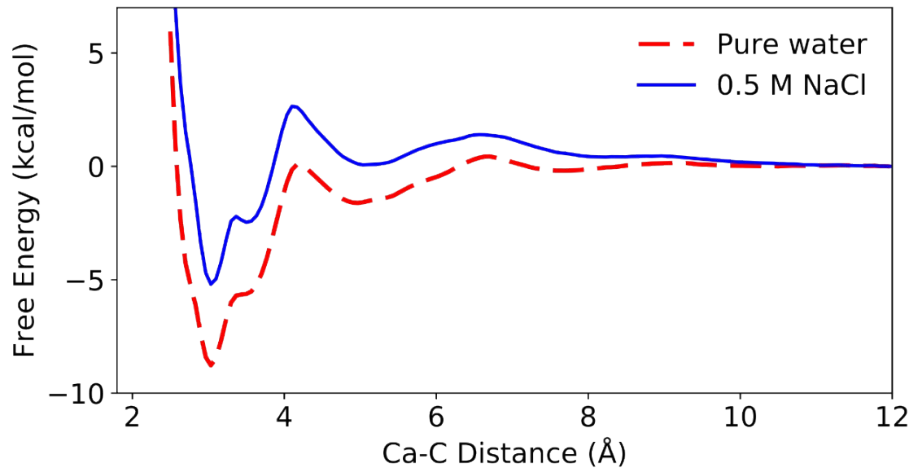

Fig. S2. Free energy profile for the association of CO_3^{2-} with Ca^{2+} in pure water and in 0.5 M NaCl.

3. Free-energy profiles for the association of Cl^- with Ca^{2+} and Mg^{2+}

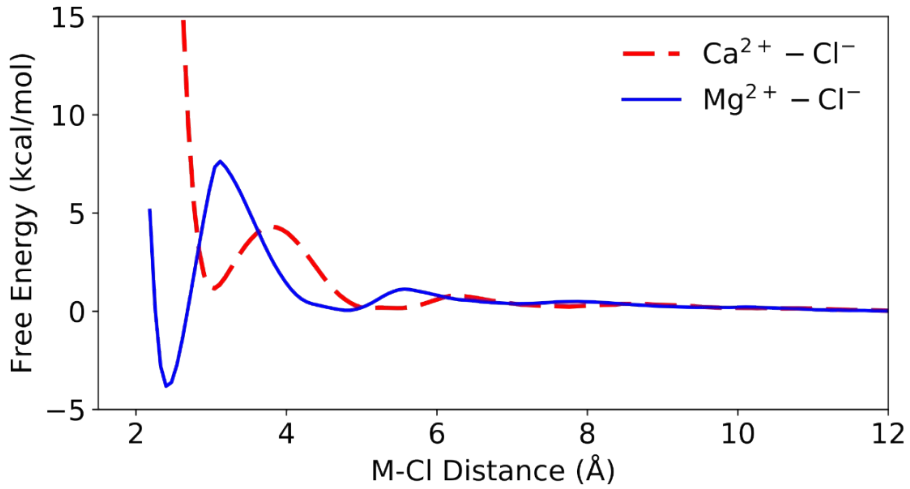

Fig. S3. Free energy profile for the association of Ca^{2+} (red dashed line) and Mg^{2+} (blue solid line) with Cl^-.