Electronic Supplementary Information for Dalton Transactions

Comparative investigation of the solution species $[U(CO_3)_5]^{6-}$ and the crystal structure of $Na_6[U(CO_3)_5]\cdot 12H_2O$

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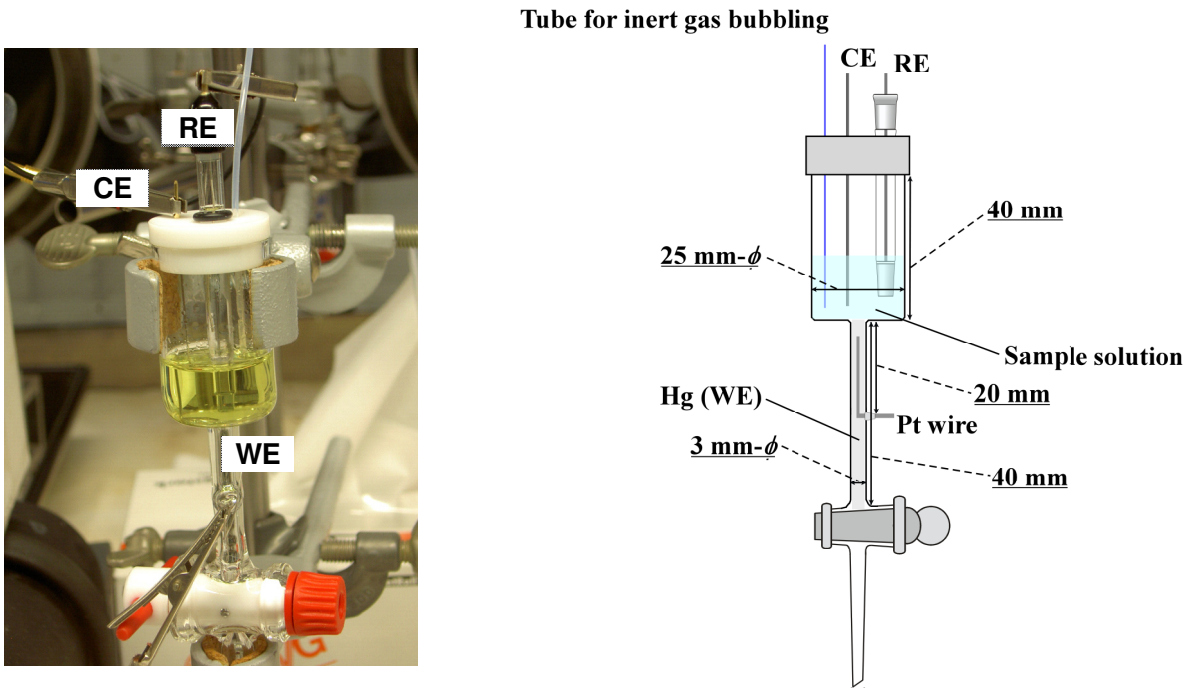

Figure S1. *Photo and electrode arrangement of electrochemical cell for electroreduction. Working electrode (WE) = Hg (Inner diameter = 3.0 mm), Counter electrode (CE) = Pt wire, Reference electrode (RE) = Ag/AgCl (with Vycor glass liguid junction). Sample volume > 2.0 ml*

<Before electrolysis (U(VI))> **<After electrolysis (U(IV))>**

Figure S2. *Color variation of uranium in 1.0 M $NaHCO_3$ before and after the electrolysis.*

Table S3. *Crystal data and structure refinement.*

Empirical formula	$Na_6[U(CO_3)_5]\cdot 12\ H_2O$
Formula weight	892.19
Temperature [K]	293(2)
Wavelength [Å]	0.71073
Crystal system, space group	triclinic, $P\bar{1}$ (No. 2)
Unit cell dimensions [Å,°]	a = 9.563(2)
	b = 9.901(2)
	c= 13.658(3)
	α = 90.452(3)
	β = 104.692(3)
	γ = 95.427(3)
Volume [$Å^3$]	1244.6(5)
Z / Calculated density [g/cm^3]	2 / 2.658
Absorption coefficient [mm^{-1}]	6.740
F(000)	856
Crystal size	0.2 x 0.14 x 0.3 mm
θ range for data collection [°]	1.54 to 30.83
Limiting indices	$-13 \le h \le 13$,
	$-13 \le k \le 14$,
	$-19 \le l \le 17$
Reflections collected / unique	9812 / 6887
R(int)	0.1258
Absorption correction	Empirical, ψ-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6887 / 0 / 353
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0690, wR2 = 0.1775
R indices (all data)	R1 = 0.0718, wR2 = 0.1807
Largest diff. peak and hole [e / $Å^3$]	5.89 and -6.68

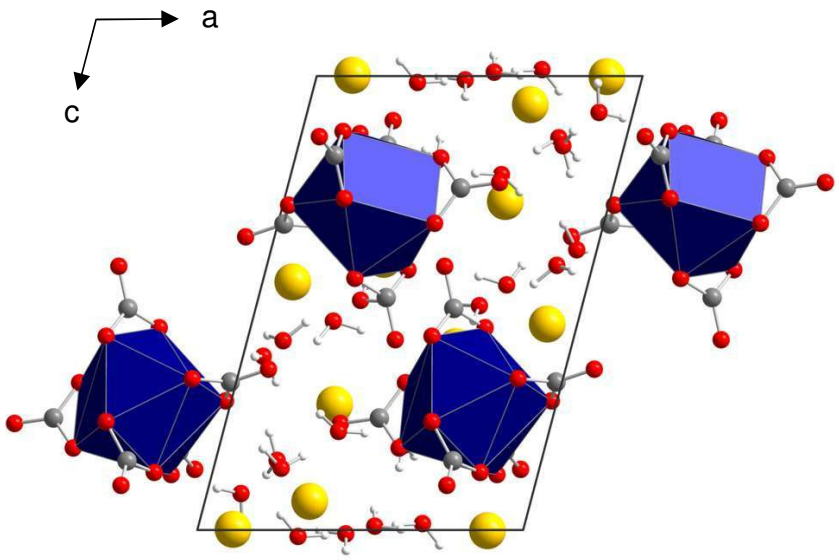

Figure S4: *Crystal structure drawn along the b-axis. The coordination polyhedron of U(IV) is blue, yellow - Na, grey - C, red - O, white - H.*

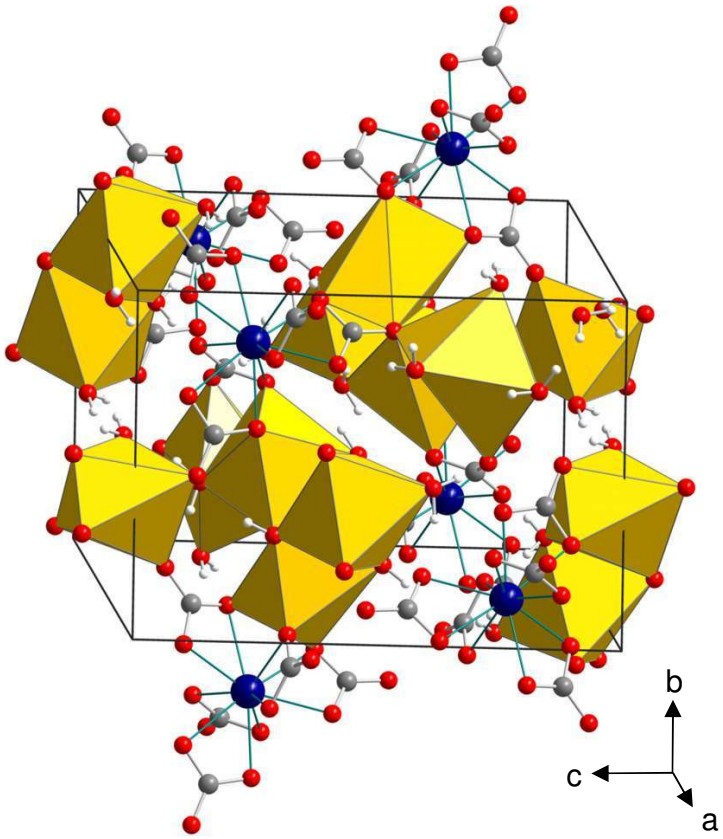

Figure S5: *The counter ion arrangement in the structure. The coordination polyhedron of Na^+ is yellow, blue - U, grey - C, red - O, white - H.*