Electronic Supplementary Material (ESI) for Dalton Transactions

Computational investigation of the speciation of uranyl gluconate complexes in aqueous solution

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Supplementary Information

Table S1: Gas-Phase ΔG_r /kJ/mol for reactions (1)–(4).

Reaction	pH	U_4 Geometry	U_5 Geometry	U_6 Geometry
1	Low	-168.35	-169.10	-177.63
2	Neutral	-55.13	-43.38	-48.13
3	High	-237.28	-224.91	-219.42
4	V. High	-272.03	-274.91	-279.96

Table S2: COSMO ΔG_r /kJ/mol for reactions (1)–(4).

Reaction	pH	U_4 Geometry	U_5 Geometry	U_6 Geometry
1	Low	-7.97	10.02	8.98
2	Neutral	-24.00	-15.73	-15.92
3	High	65.22	90.96	73.04
4	V. High	2.98	-38.13	-37.29

Table S3: Experimental and calculated ^{13}C NMR chemical shifts δ/ppm for D-gluconic acid and $UO_2Glu(H_2O)(OH)_2^-$ in the U_4, U_5 and U_6 geometries. MAD = Mean absolute deviation (see Fig. 1 for atom labelling).

Species	C_1	C_2	C_3	C_4	C_5	C_6	MAD
Experimental[19] D-gluconic acid pH 7	178.8	74.1	71.0	72.5	71.2	62.6	
This work, D-gluconate ion	176.2	84.5	78.1	93.8	81.1	72.3	
Absolute deviation	2.6	10.4	7.2	21.3	9.9	9.7	10.2
Experimental[19] Uranyl gluconate pH 11	191.0	88.5	85.6	77.7	74.4	65.1	
This work, $UO_2Glu(H_2O)(OH)_2^-$ U_4	186.2	84.9	76.9	83.5	75.9	69.3	
Absolute deviation	4.8	3.6	8.7	5.8	1.5	4.2	4.8
This work $UO_2Glu(H_2O)(OH)_2^-$ U_5	177.8	80.9	77.8	83.8	75.6	68.7	
Absolute Deviation	13.2	7.6	7.8	6.1	1.2	3.6	6.6
This work $UO_2Glu(H_2O)(OH)_2^-$ U_6	179.1	80.9	82.5	80.9	79.6	63.6	
Absolute Deviation	11.9	7.6	3.1	3.2	5.2	1.5	5.4

Table S4: COSMO calculated ΔG_r kJ/mol for 1:2 Uranyl D-gluconate complexes

	Glu 1 / Glu 2 coordination ΔG_r kJ/mol			
Reaction	U_4 / U_4	U_5 / U_5	U_6 / U_6	U_5 / U_4
7	44.97	48.03	31.99	
8	-34.70	-21.73	-35.44	
9	99.30	94.61	99.02	
10		149.21		128.70
11		79.27		62.86
12				170.40
13				90.73

Table S5: COSMO calculated ΔG_r /kJ/mol for 1:3 $UO_2Glu_3^-$ complexes

Reaction	pH	U_4 Geometry	U_5 Geometry	U_6 Geometry
14	Low	116.28	128.92	138.29
15	Neutral	20.59	33.23	42.59
16	High	-1.78	10.86	20.22