Is gluconate a good model for isosaccharinate in uranyl(VI) chemistry? A DFT study.

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Supporting 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	-146.10	-191.95	-121.53
2	Neutral	-7.67	-35.22	-3.71
3	High	-159.11	-119.62	-124.40
4	V. High	-226.60	-231.17	-166.23

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

Reaction	pH	U_4 Geometry	U_5 Geometry	U_6 Geometry
1	Low	5.03	-1.79	32.49
2	Neutral	-6.54	-5.77	10.01
3	High	76.75	93.28	102.08
4	V. High	-17.38	-52.09	-60.25

Table S3: H-bonding interaction distances (Å) between the Isa ligand and uranyl for COSMO uranyl-Isa optimised geometries. See Fig. 1 for labelling. O_{solv} = oxygen in the primary solvation shell. O_{ax} = uranyl oxygen, n/a = no H-bonding between the Isa ligand and uranyl.

Reaction	U_4 geometry		U_5 geometry		U_6 geometry	
	Distance	Description	Distance	Description	Distance	Description
1	n/a	n/a	1.627	H_4-O_{solv}	n/a	n/a
2	n/a	n/a	2.079	H_5-O_{ax}	n/a	n/a
3	2.030	H_3-O_{ax}	1.679	H_5-O_{solv}	n/a	n/a
4	n/a	n/a	1.820	H_5-O_{solv}	n/a	n/a
4b	n/a	n/a	1.634	H_5-O_{solv}	n/a	n/a

Table S4: COSMO ΔG_r /kJ/mol for reactions (7)–(13), 1:2 uranyl-Isa complexes

Reaction	U_4 Geometry	U_5 Geometry	U_6 Geometry
7	59.19	60.29	49.84
8	-24.94	-31.43	-23.38
9	114.99	97.52	107.78
10	-	167.09	138.07
11	-	-0.48	-23.40
12	138.06	183.99	152.04
13	53.93	16.42	-9.42

Table S5: COSMO ΔG_r /kJ/mol for reactions (14)–(16), 1:3 $UO_2Isa_3^-$ complexes

Reaction	U_4 Geometry	U_5 Geometry	U_6 Geometry
14	131.48	168.79	156.85
15	35.78	73.09	61.15
16	13.41	50.72	38.78