Supporting Information

Studies of the Complexation of Gluconate with Th(IV) in Acidic Solutions: Stability Constant Determination and Coordination Mode Analysis

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Table S1 Initial conditions and concentration analyses of pD titration solutions

Sample ID	Initial Condition					Concentration Analysis			
	V mL	$C_{Th(total)}$ mmol.L^{-1}	$C_{G(total,init)}$ mmol.L^{-1}	$C_{D(total,init)}$ mmol.L^{-1}	$C_{NO3(total)}$ mmol.L^{-1}	C_A mmol.L^{-1}	I_A	I_G	$C_{G(total)}$ mmol.L^{-1}
ThG1-1	10.66	41.69	41.7	4.63	0	3.60	1.00	3.86	41.7
ThG1-2	10.71	41.49	41.5	6.83	1.83	3.58	1.00	3.83	41.1
ThG1-3	10.76	41.30	41.3	9.00	3.64	3.56	1.00	3.72	39.7
ThG1-4	10.81	41.11	41.1	11.2	5.44	3.55	1.00	3.59	38.2
ThG1-5	10.86	40.92	40.9	13.3	7.22	3.53	1.00	3.47	36.8
ThG3-1	10.82	40.84	40.8	15.5	9.04	3.54	1.00	3.34	35.5
ThG3-2	10.87	40.65	40.7	17.6	10.82	3.52	1.00	3.24	34.2
ThG3-3	10.92	40.47	40.5	19.7	12.55	3.51	1.00	3.11	32.8
ThG3-4	10.96	40.30	40.3	21.6	14.12	3.49	1.00	3.00	31.4
ThG3-5	11.01	40.12	40.1	23.6	15.83	3.48	1.00	2.88	30.1
ThG2-1	11.60	38.21	38.2	24.7	16.90	3.30	1.00	2.86	28.3
ThG2-2	11.80	37.56	37.6	28.3	19.93	3.25	1.00	2.81	27.4
ThG2-3	12.00	36.94	36.9	31.8	22.87	3.19	1.00	2.78	26.6
ThG2-4	12.20	36.33	36.3	35.2	25.71	3.14	1.00	2.74	25.8
ThG2-5	12.40	35.75	35.8	38.5	28.46	3.09	1.00	2.70	25.0

Table S2 Estimation of the variation in the complexation constants of GH_2^{3-} with Th^{4+} and $Th(OH)_2^{2+}$.

Reaction	Step reaction	Equilibrium Constant
$Th^{4+} + GH_4^- = Th(GH_2)^+ + 2H^+$ ($\log \beta_{101(-2)} = -2.3$)	$GH_4^- = GH_2^{3-} + 2H^+$ $Th^{4+} + GH_2^{3-} = Th(GH_2)^+$	Log K_d (unknown) Log $K_{(Th/GH2)} = \log \beta_{101(-2)} - \log K_d$ $= (-2.3) - \log K_d$
$Th^{4+} + GH_4^- + 2H_2O =$ $Th(OH)_2(GH_2)^- + 4H^+$ ($\log \beta_{1-21(-2)} = -13.9$)	$GH_4^- = GH_2^{3-} + 2H^+$ $Th^{4+} + 2H_2O = Th(OH)_2^{2+} + 2H^+$ $Th(OH)_2^{2+} + GH_2^{3-} = Th(OH)_2(GH_2)^-$	Log K_d (unknown) Log $K_{(Th/(OH)2)} = -8.6$[a] Log $K_{(Th/(OH)2/GH2)}$ $= \log \beta_{1-21(-2)} - \log K_d - \log K_{(Th/(OH)2)}$ $= -5.3 - \log K_d$
Difference between $\log K_{(Th/GH2)}$ & $\log K_{(Th/(OH)2/GH2)}$	$\Delta \log K =$ $\log K_{(Th/GH2)} - \log K_{(Th/(OH)2/GH2)}$	$\Delta \log K = (-2.3) – (-5.3)$ $= 3.0$

[a] this value was from the reference [23].