Equilibrium, kinetic and solvent effect studies on the reactions of [Ru^{III}(Hedta)H$_2$O] with thiols

Mohamed M. Shoukry, Mohamed R. Shehata, Mohamed S. A. Hamza

and Rudi van Eldik*

Table SI-1. Acid-base data for Ru^{III}(edta)(H$_2$O)$^-$ at different concentrations of dioxane at 25 °C and 0.1 M ionic strength.

Dioxane (%)	M	H[a]	logβ[b]
0	1	1	3.12(0.01)
	1	-1	-7.41(0.02)
12.5	1	1	3.21(0.02)
	1	-1	-7.50(0.03)
25	1	1	3.34(0.02)
	1	-1	-7.74(0.04)
37.5	1	1	3.48(0.03)
	1	-1	-7.97(0.04)
50	1	1	3.62(0.02)
	1	-1	-8.15(0.03)
62.5	1	1	3.72(0.04)
	1	-1	-8.31(0.05)

[a] M and H are the stoichiometric coefficients corresponding to Ru^{III}(edta)(H$_2$O)$^-$ and H$^+$, respectively. [b] Standard deviations are given in parentheses; sum of square of residuals are less than 5 x 10^{-7}.

Table SI-2. Complex-formation constants for $Ru^{III}(edta)(H_2O)^-$ with 2-aminoethanethiol.HCl at different concentrations of dioxane at 25 °C and 0.1 M ionic strength.

Dioxane (%)	M	L	H[a]	$\log\beta$[b]	pK_a
0	1	1	0	10.36(0.02)	
	1	1	1	18.33(0.04)	7.97
12.5	1	1	0	10.79(0.03)	
	1	1	1	18.64 (0.04)	7.85
25	1	1	0	11.31 (0.04)	
	1	1	1	18.97(0.05)	7.66
37.5	1	1	0	11.71(0.03)	
	1	1	1	19.24(0.04)	7.53
50	1	1	0	12.27(0.04)	
	1	1	1	19.53(0.05)	7.26
62.5	1	1	0	12.44(0.04)	
	1	1	1	19.62(0.06)	7.18

[a] M, L and H are the stoichiometric coefficients corresponding to $Ru^{III}(edta)(H_2O)^-$, Ligand and H^+, respectively. [b] Standard deviations are given in parentheses; sum of square of residuals are less than 5 x 10^{-7}.

Table SI-3. Acid-base data for mercaptoacetic acid at different concentrations of dioxane at 25 °C and 0.1 M ionic strength.

Dioxane (%)	L	H[a]	$\log\beta$[b]	pK_a
0	1	1	10.07(0.02)	10.07
	1	2	13.58(0.03)	3.51
12.5	1	1	10.49(0.02)	10.49
	1	2	14.51(0.02)	4.02
25	1	1	11.10(0.02)	10.49
	1	2	15.19(0.04)	4.09
37.5	1	1	11.45(0.03)	11.45
	1	2	16.02(0.03)	4.57
50	1	1	11.98(0.03)	11.98
	1	2	16.81(0.04)	4.83
62.5	1	1	11.98(0.04)	11.98
	1	2	17.59(0.05)	5.24

[a] L and H are the stoichiometric coefficients corresponding to Ligand and H^+, respectively. [b] Standard deviations are given in parentheses; sum of square of residuals are less than 5×10^{-7}.

Table SI-4. Complex-formation constants for $Ru^{III}(edta)(H_2O)^-$ with mercaptoacetic acid for different concentrations of dioxane at 25 °C and 0.1 M ionic strength.

Dioxane (%)	M	L	H[a]	$\log\beta$[b]	pK_a
0	1	1	0	9.86(0.03)	
	1	1	1	13.92(0.04)	4.06
12.5	1	1	0	10.32(0.02)	
	1	1	1	14.25(0.03)	3.93
25	1	1	0	10.69(0.04)	
	1	1	1	14.59(0.05)	3.90
37.5	1	1	0	11.14(0.03)	
	1	1	1	14.89(0.05)	3.75
50	1	1	0	11.55(0.02)	
	1	1	1	15.23(0.04)	3.68
62.5	1	1	0	11.73(0.04)	
	1	1	1	15.19(0.06)	3.46

[a] M, L and H are the stoichiometric coefficients corresponding to $Ru^{III}(edta)(H_2O)^-$, Ligand and H^+, respectively. [b] Standard deviations are given in parentheses; sum of square of residuals are less than 5×10^{-7}.
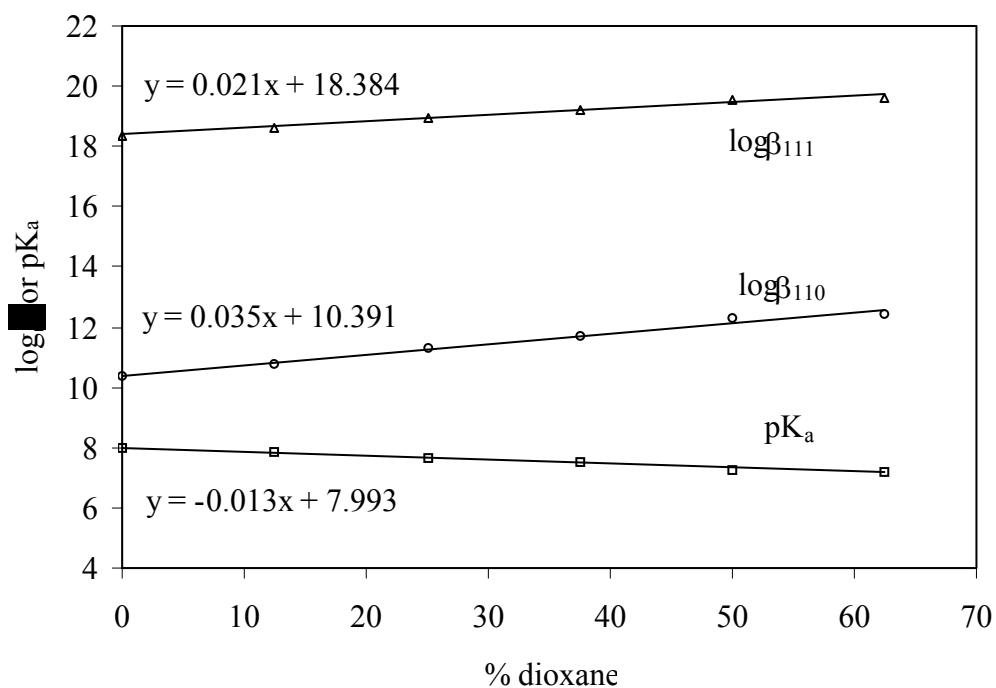
Figure SI-1. Complex-formation constants for $Ru^{III}(edta)(H_2O)^-$ with 2-aminoethanethiol.HCl at different concentrations of dioxane, pK_a of protonated complex ($logB_{111}$-$log B_{110}$)
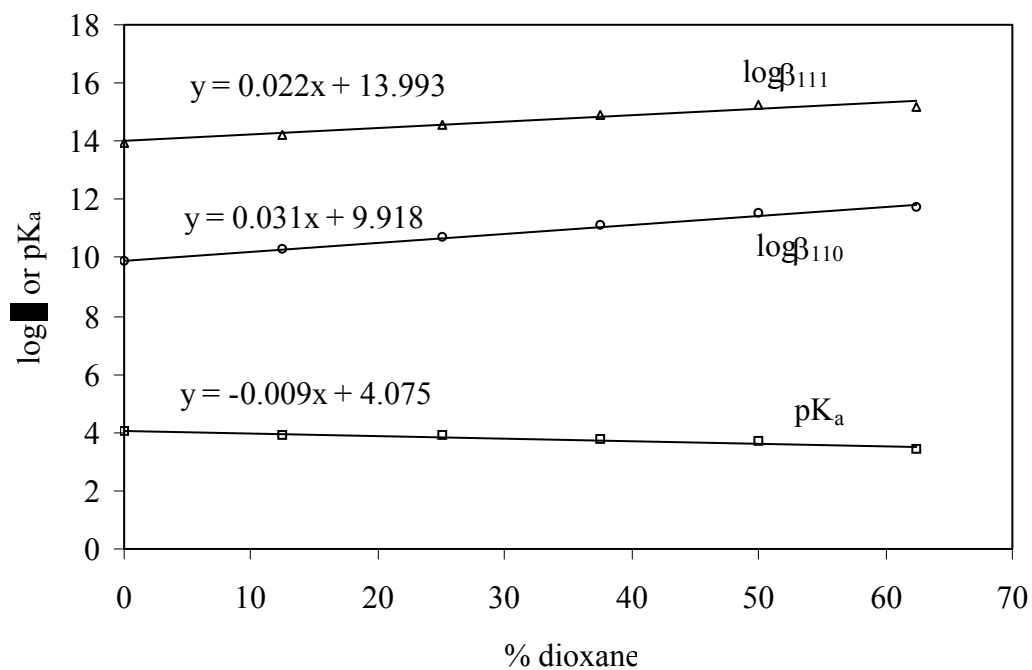
Figure SI-2. Complex-formation constants for $Ru^{III}(edta)(H_2O)^-$ with mercaptoacetic acid at different concentrations of dioxane , pK_a of protonated complex $(\log B_{111} - \log B_{110})$.