

Np(V) complexation with propionate in 0.1 – 4 M NaCl solutions at

20–85°C†

Supporting information

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Table caption

Table S1: Stability constants for the formation of 1:1 complex ($\text{NpO}_2^+ + \text{Prop}^- = \text{NpO}_2(\text{Prop})$) measured in 0.51 m NaCl solution as a function of temperature (23–85 °C), and extrapolated to $I = 0$.

Table S2: Composition of EXAFS samples 1-4.

Temperature /°C	[NaCl] / molal	Log $\beta_0(T)$ Average $\pm 1\sigma$
20	0.506	1.33 \pm 0.10
23	0.506	1.26 \pm 0.07
23	0.506	1.31 \pm 0.06
40	0.506	1.41 \pm 0.10
60	0.506	1.48 \pm 0.10
70	0.506	1.57 \pm 0.10
85	0.506	1.67 \pm 0.13

Table S1

Sample	[Np(V)] / mmol/L	[propionate ⁻] / mol/L	pH _c	[NaCl] / molal
1	0.77	0.48	5.5	0.51
2	0.77	0.48	5.1	1.02
3	0.77	0.48	5.0	2.09
4	0.77	0.48	5.0	4.37

Table S2

Figure caption

Figure S1:(a) Np(V) absorption spectra for various propionate concentration ($I = 0.51\text{m}$; $T = 85^\circ\text{C}$, $\text{pH}_c = 5.0$). (b) Example of a deconvoluted spectrum ($[\text{Prop}] = 0.10\text{m}$; $I = 0.51\text{m}$; $\text{pH}_c = 5.0$, $T = 85^\circ\text{C}$).

Figure S2:(a) Np(V) absorption spectra for various propionate concentration ($I = 3.14\text{ m}$; $T = 23^\circ\text{C}$, $\text{pH}_c = 5.0$). (b) Example of a deconvoluted spectrum ($[\text{Prop}] = 0.14\text{ m}$; $I = 3.2\text{ m}$; $\text{pH}_c = 5.0$, $T = 23^\circ\text{C}$).

Figure S3:Np(V) absorption spectra for NpO_2^+ aqueous ion and the EXAFS sample 1 ($I = 0.51\text{ m}$; $T = 23^\circ\text{C}$, $\text{pH}_c = 5.0$, $[\text{Prop}]_{\text{tot}} = 0.48\text{ M}$). Deconvolution of the later spectrum shows that approximately 95% of the $\text{NpO}_2(\text{Prop})$ complex is formed.

Figure S4: Possible structural scheme of Np(V)-propionate complex in the solution a) Bidentate mode b) Monodentate mode.

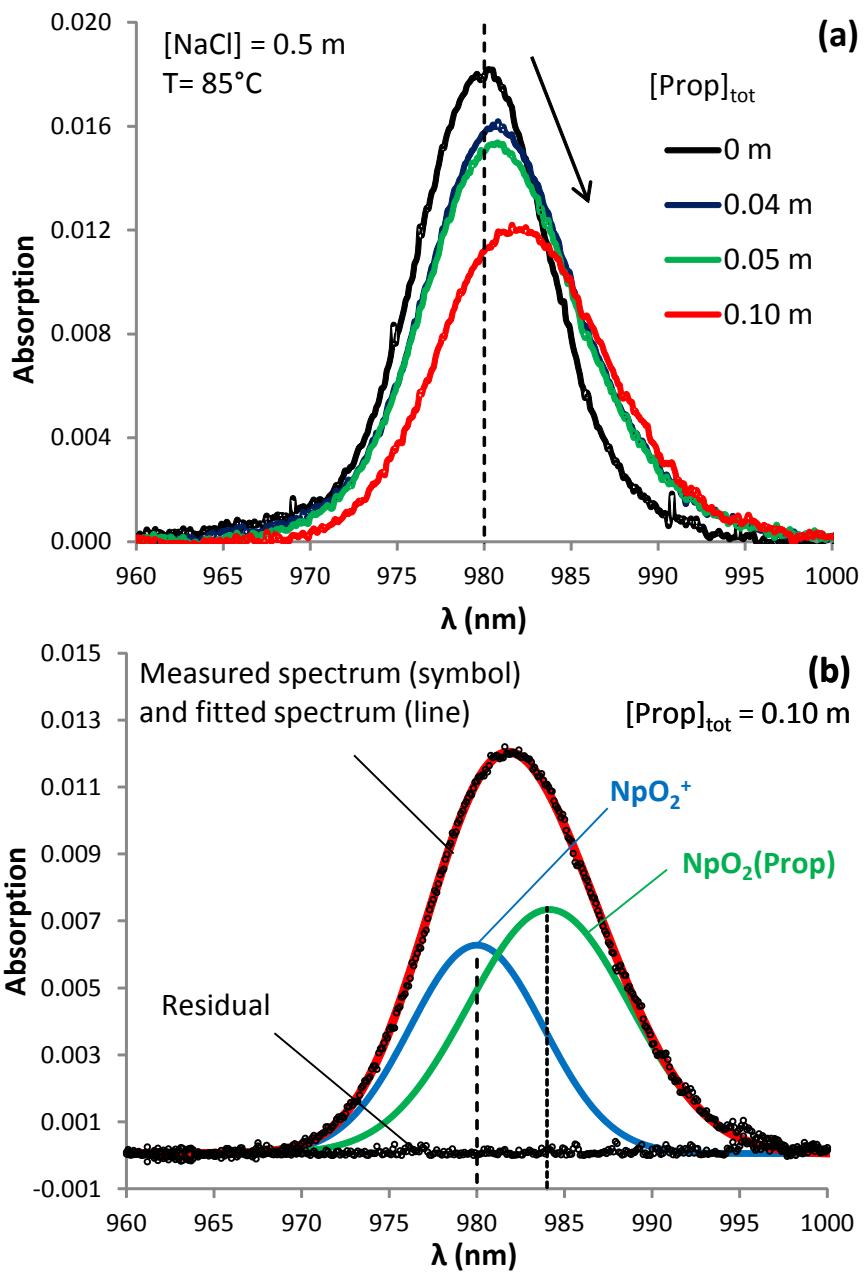


Figure S1

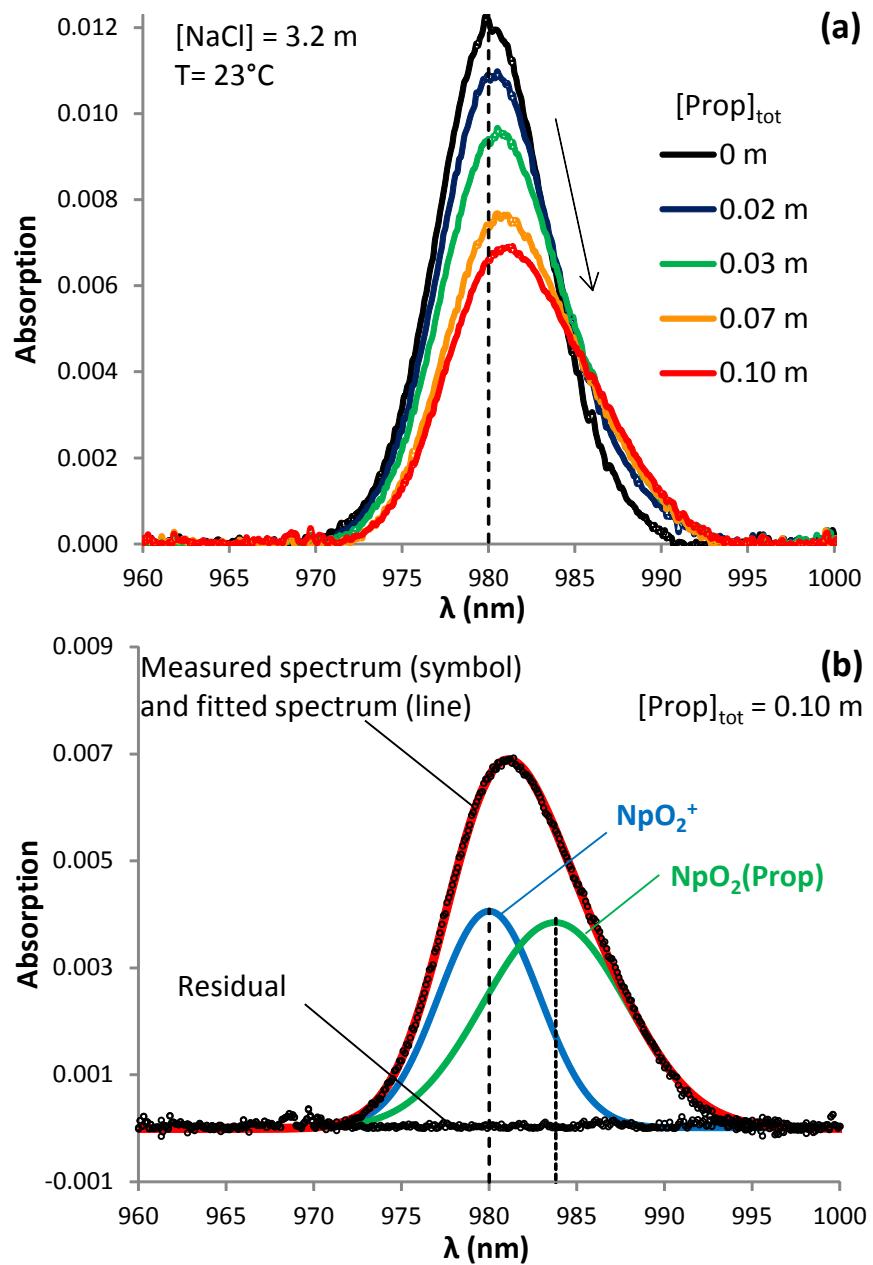


Figure S2

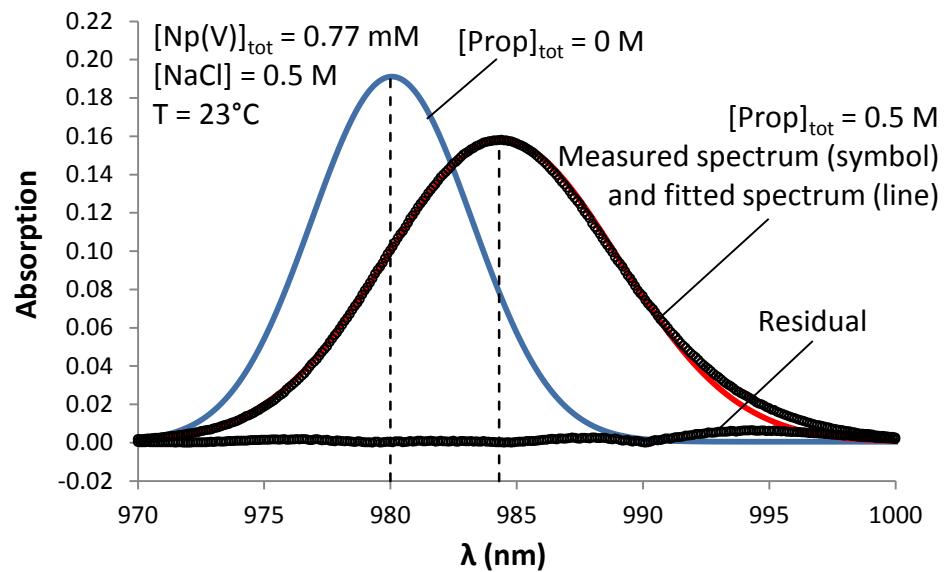
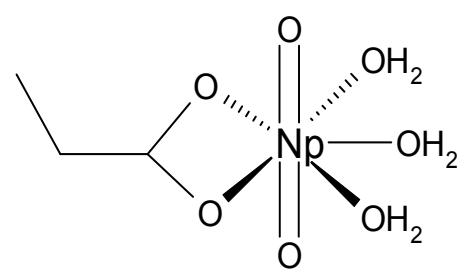
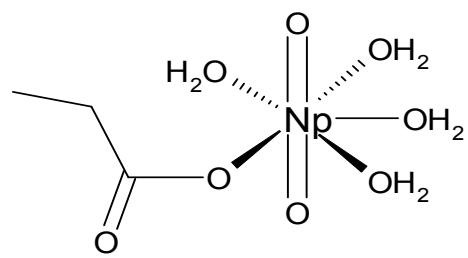


Figure S3



a)



b)

Figure S4