Speciation, thermodynamics and structure of Np(V) oxalate complexes in aqueous solution

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Supporting Information

Figures:

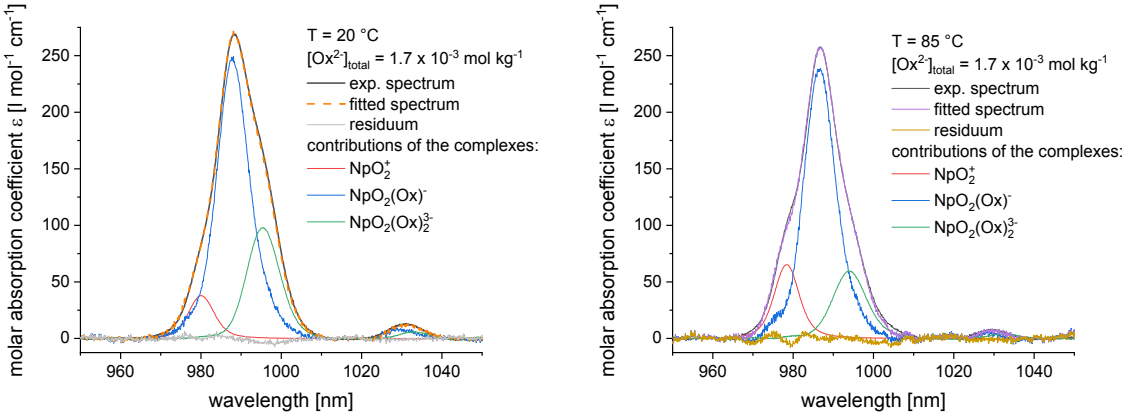

Figure S1: exemplary deconvolution of the absorption spectra of Np(V) at $[Ox^{2-}]_{total}$ = 1.7 x 10^{-3} mol kg^{-1} at T = 20 (left) and 85 °C (right) and $I_m(NaClO_4)$ = 1.0 mol kg^{-1}; $[H^+]_{total}$ = 2.1 x 10^{-5} mol kg^{-1}; $[NpO_2^+]_{total}$ = 2.5 x 10^{-4} mol kg^{-1}.

Tables

Sample compositions of the performed absorption spectroscopic measurements

Sample compositions for the determination of the complex stoichiometry as a function of the oxalate concentration at a fixed ionic strength I_m.

Table S1: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 20 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m ($NaClO_4$)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.20E-05	1.80E-04	0.5	0.49	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	7.67E-06	4.32E-04	0.23	0.68	0.08
4	2.49E-04	1.66E-03	2.08E-05	1.00	4.68E-06	8.67E-04	0.1	0.71	0.24
5	2.48E-04	2.49E-03	2.08E-05	1.00	3.38E-06	1.30E-03	0.05	0.61	0.36
8	2.47E-04	3.31E-03	2.07E-05	1.00	2.64E-06	1.73E-03	0.03	0.55	0.44
7	2.46E-04	4.39E-03	2.07E-05	1.00	2.05E-06	2.30E-03	0.02	0.48	0.52
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.60E-06	3.01E-03	0.01	0.41	0.59
9	2.43E-04	7.59E-03	2.07E-05	1.00	1.23E-06	3.98E-03	0	0.37	0.69
10	2.41E-04	1.05E-02	2.06E-05	0.99	9.05E-07	5.49E-03	0.01	0.3	0.73
11	2.37E-04	1.43E-02	2.06E-05	0.99	6.68E-07	7.50E-03	0	0.25	0.75

Table S2: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 30 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m ($NaClO_4$)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.77E-04	1.77E-04	0.51	0.48	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	7.41E-06	4.24E-04	0.24	0.68	0.08
4	2.49E-04	1.66E-03	2.08E-05	1.00	4.50E-06	8.51E-04	0.1	0.73	0.23
5	2.48E-04	2.49E-03	2.08E-05	1.00	3.23E-06	1.28E-03	0.05	0.63	0.34
8	2.47E-04	3.31E-03	2.07E-05	1.00	2.52E-06	1.70E-03	0.03	0.57	0.42
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.95E-06	2.26E-03	0.01	0.5	0.51
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.53E-06	2.95E-03	0	0.44	0.58
9	2.43E-04	7.59E-03	2.07E-05	1.00	1.17E-06	3.91E-03	0	0.4	0.68
10	2.41E-04	1.05E-02	2.06E-05	0.99	8.60E-07	5.39E-03	0	0.3	0.71
11	2.37E-04	1.43E-02	2.06E-05	0.99	6.35E-07	7.36E-03	0	0.25	0.76

Table S3: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 40 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.14E-05	1.73E-04	0.51	0.47	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	7.10E-06	4.14E-04	0.25	0.69	0.06
4	2.49E-04	1.66E-03	2.08E-05	1.00	4.27E-06	8.30E-04	0.1	0.75	0.2
5	2.48E-04	2.49E-03	2.08E-05	1.00	3.05E-06	1.25E-03	0.05	0.68	0.28
8	2.47E-04	3.31E-03	2.07E-05	1.00	2.38E-06	1.66E-03	0.02	0.62	0.37
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.84E-06	2.20E-03	0.01	0.56	0.45
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.43E-06	2.88E-03	0	0.49	0.52
9	2.43E-04	7.59E-03	2.07E-05	1.00	1.10E-06	3.82E-03	0	0.45	0.62
10	2.41E-04	1.05E-02	2.06E-05	0.99	8.07E-07	5.27E-03	0	0.34	0.65
11	2.37E-04	1.43E-02	2.06E-05	0.99	5.95E-07	7.19E-03	0	0.3	0.7

Table S4: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 50 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.10E-05	1.69E-04	0.53	0.45	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	6.77E-06	4.04E-04	0.25	0.68	0.06
4	2.49E-04	1.66E-03	2.08E-05	1.00	4.03E-06	8.12E-04	0.1	0.75	0.19
5	2.48E-04	2.49E-03	2.08E-05	1.00	2.87E-06	1.22E-03	0.05	0.66	0.29
8	2.47E-04	3.31E-03	2.07E-05	1.00	2.23E-06	1.62E-03	0.01	0.62	0.37
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.72E-06	2.16E-03	0	0.54	0.47
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.34E-06	2.82E-03	0	0.47	0.54
9	2.43E-04	7.59E-03	2.07E-05	1.00	1.03E-06	3.73E-03	0	0.42	0.65
10	2.41E-04	1.05E-02	2.06E-05	0.99	7.53E-07	5.15E-03	0	0.31	0.68
11	2.37E-04	1.43E-02	2.06E-05	0.99	5.55E-07	7.03E-03	0	0.25	0.75

Table S5: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 60 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.06E-05	1.64E-04	0.57	0.42	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	6.41E-06	3.95E-04	0.31	0.64	0.05
4	2.49E-04	1.66E-03	2.08E-05	1.00	3.77E-06	7.93E-04	0.15	0.74	0.17
5	2.48E-04	2.49E-03	2.08E-05	1.00	2.68E-06	1.19E-03	0.08	0.67	0.27
8	2.47E-04	3.31E-03	2.07E-05	1.00	2.08E-06	1.58E-03	0.05	0.63	0.34
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.60E-06	2.11E-03	0.03	0.57	0.43
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.24E-06	2.75E-03	0.02	0.51	0.5
9	2.43E-04	7.59E-03	2.07E-05	1.00	9.51E-07	3.65E-03	0.02	0.46	0.6
10	2.41E-04	1.05E-02	2.06E-05	0.99	6.97E-07	5.03E-03	0.01	0.35	0.64
11	2.37E-04	1.43E-02	2.06E-05	0.99	5.13E-07	6.87E-03	0.01	0.31	0.7

Table S6: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 70 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	1.02E-05	1.60E-04	0.57	0.41	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	6.02E-06	3.85E-04	0.32	0.62	0.05
4	2.49E-04	1.66E-03	2.08E-05	1.00	3.51E-06	7.73E-04	0.17	0.75	0.16
5	2.48E-04	2.49E-03	2.08E-05	1.00	2.47E-06	1.16E-03	0.09	0.69	0.25
8	2.47E-04	3.31E-03	2.07E-05	1.00	1.91E-06	1.54E-03	0.06	0.64	0.33
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.47E-06	2.05E-03	0.04	0.59	0.41
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.14E-06	2.68E-03	0.02	0.53	0.48
9	2.43E-04	7.59E-03	2.07E-05	1.00	8.73E-07	3.56E-03	0.02	0.49	0.57
10	2.41E-04	1.05E-02	2.06E-05	0.99	6.39E-07	4.90E-03	0.01	0.38	0.61
11	2.37E-04	1.43E-02	2.06E-05	0.99	4.70E-07	6.69E-03	0	0.33	0.67

Table S7 sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 80 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	9.69E-06	1.56E-04	0.6	0.41	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	5.63E-06	3.76E-04	0.33	0.64	0.05
4	2.49E-04	1.66E-03	2.08E-05	1.00	3.24E-06	7.56E-04	0.18	0.75	0.16
5	2.48E-04	2.49E-03	2.08E-05	1.00	2.28E-06	1.13E-03	0.1	0.71	0.24
8	2.47E-04	3.31E-03	2.07E-05	1.00	1.76E-06	1.51E-03	0.07	0.68	0.3
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.35E-06	2.01E-03	0.05	0.61	0.39
8	2.45E-04	5.73E-03	2.07E-05	1.00	1.05E-06	2.63E-03	0.03	0.57	0.46
9	2.43E-04	7.59E-03	2.07E-05	1.00	7.98E-07	3.48E-03	0.02	0.51	0.55
10	2.41E-04	1.05E-02	2.06E-05	0.99	5.84E-07	4.80E-03	0.01	0.41	0.59
11	2.37E-04	1.43E-02	2.06E-05	0.99	4.29E-07	6.55E-03	0.01	0.35	0.65

Table S8: sample composition for the determination of the complex stoichiometry as a function of $[Ox^{2-}]_{total}$ at I_m = 1.0 mol kg^{-1} $NaClO_4$ and T = 85 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	2.51E-04	0.00E+00	2.08E-05	1.00	2.08E-05	0.00E+00	1	0	0
2	2.51E-04	3.51E-04	2.08E-05	1.00	9.32E-06	1.50E-04	0.6	0.4	0
3	2.50E-04	8.35E-04	2.08E-05	1.00	5.33E-06	3.61E-04	0.35	0.65	0.05
4	2.49E-04	1.66E-03	2.08E-05	1.00	3.04E-06	7.25E-04	0.18	0.77	0.15
5	2.48E-04	2.49E-03	2.08E-05	1.00	2.13E-06	1.09E-03	0.1	0.73	0.23
8	2.47E-04	3.31E-03	2.07E-05	1.00	1.64E-06	1.45E-03	0.07	0.7	0.3
7	2.46E-04	4.39E-03	2.07E-05	1.00	1.26E-06	1.93E-03	0.05	0.63	0.38
8	2.45E-04	5.73E-03	2.07E-05	1.00	9.75E-07	2.52E-03	0.03	0.57	0.45
9	2.43E-04	7.59E-03	2.07E-05	1.00	7.43E-07	3.34E-03	0.03	0.53	0.54
10	2.41E-04	1.05E-02	2.06E-05	0.99	5.43E-07	4.60E-03	0.02	0.43	0.58
11	2.37E-04	1.43E-02	2.06E-05	0.99	3.99E-07	6.28E-03	0.01	0.37	0.64

Sample compositions for the determination of ionic strength effects for the complexation of Np(V) with oxalate as a function of the ionic strength I_m at fixed oxalate concentrations.

Used background electrolyte: $NaClO_4$

Table S9: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 20 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	1.15E-06	3.25E-03	0.01	0.49	0.49
2	1.73E-04	5.29E-03	1.78E-05	0.68	1.32E-06	3.00E-03	0.01	0.46	0.53
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.45E-06	2.81E-03	0.01	0.44	0.55
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.55E-06	2.66E-03	0.01	0.41	0.58
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.63E-06	2.52E-03	0.01	0.40	0.59
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.69E-06	2.41E-03	0.01	0.38	0.61
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.72E-06	2.31E-03	0.01	0.36	0.63
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.74E-06	2.22E-03	0.01	0.35	0.64

Table S10: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 30 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	1.09E-06	3.19E-03	0.01	0.50	0.49
2	1.73E-04	5.29E-03	1.78E-05	0.68	1.25E-06	2.95E-03	0.01	0.48	0.51
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.38E-06	2.76E-03	0.01	0.45	0.54
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.48E-06	2.61E-03	0.01	0.43	0.56
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.56E-06	2.48E-03	0.01	0.41	0.58
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.61E-06	2.37E-03	0.01	0.39	0.60
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.64E-06	2.27E-03	0.01	0.37	0.62
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.66E-06	2.18E-03	0.01	0.36	0.63

Table S11: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 40 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	1.02E-06	3.13E-03	0.00	0.56	0.44
2	1.73E-04	5.29E-03	1.78E-05	0.68	1.17E-06	2.88E-03	0.00	0.53	0.47
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.30E-06	2.70E-03	0.00	0.51	0.49
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.39E-06	2.55E-03	0.00	0.48	0.52
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.47E-06	2.42E-03	0.00	0.47	0.53
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.52E-06	2.31E-03	0.00	0.45	0.55
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.55E-06	2.21E-03	0.00	0.43	0.57
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.57E-06	2.13E-03	0.00	0.42	0.58

Table S12: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 50 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	9.43E-07	3.06E-03	0.00	0.55	0.45
2	1.73E-04	5.29E-03	1.78E-05	0.68	1.09E-06	2.82E-03	0.00	0.52	0.48
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.21E-06	2.64E-03	0.00	0.48	0.52
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.30E-06	2.49E-03	0.00	0.46	0.54
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.37E-06	2.36E-03	0.00	0.45	0.55
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.42E-06	2.25E-03	0.00	0.43	0.57
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.46E-06	2.16E-03	0.00	0.41	0.59
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.47E-06	2.08E-03	0.00	0.40	0.60

Table S13: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 60 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	8.69E-07	3.00E-03	0.02	0.57	0.41
2	1.73E-04	5.29E-03	1.78E-05	0.68	1.01E-06	2.76E-03	0.02	0.54	0.44
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.12E-06	2.58E-03	0.02	0.52	0.46
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.21E-06	2.43E-03	0.02	0.51	0.47
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.28E-06	2.31E-03	0.02	0.48	0.50
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.33E-06	2.20E-03	0.02	0.46	0.52
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.36E-06	2.11E-03	0.02	0.45	0.53
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.37E-06	2.03E-03	0.02	0.43	0.55

Table S14: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 70 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	7.93E-07	2.93E-03	0.02	0.59	0.39
2	1.73E-04	5.29E-03	1.78E-05	0.68	9.27E-07	2.69E-03	0.02	0.56	0.42
3	1.70E-04	5.22E-03	1.78E-05	0.87	1.03E-06	2.51E-03	0.02	0.54	0.44
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.11E-06	2.37E-03	0.02	0.52	0.46
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.18E-06	2.25E-03	0.02	0.50	0.48
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.22E-06	2.15E-03	0.02	0.48	0.49
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.25E-06	2.06E-03	0.02	0.46	0.52
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.27E-06	1.97E-03	0.02	0.46	0.52

Table S15: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 80 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	7.21E-07	2.87E-03	0.02	0.60	0.38
2	1.73E-04	5.29E-03	1.78E-05	0.68	8.45E-07	2.63E-03	0.02	0.58	0.40
3	1.70E-04	5.22E-03	1.78E-05	0.87	9.42E-07	2.46E-03	0.02	0.57	0.41
4	1.68E-04	5.14E-03	1.78E-05	1.07	1.02E-06	2.32E-03	0.02	0.54	0.44
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.08E-06	2.20E-03	0.03	0.52	0.45
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.13E-06	2.10E-03	0.03	0.51	0.46
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.15E-06	2.01E-03	0.03	0.48	0.48
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.17E-06	1.94E-03	0.03	0.47	0.49

Table S16: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 85 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	5.36E-03	1.78E-05	0.49	6.69E-07	2.77E-03	0.03	0.61	0.37
2	1.73E-04	5.29E-03	1.78E-05	0.68	7.86E-07	2.54E-03	0.03	0.59	0.38
3	1.70E-04	5.22E-03	1.78E-05	0.87	8.77E-07	2.36E-03	0.03	0.57	0.40
4	1.68E-04	5.14E-03	1.78E-05	1.07	9.51E-07	2.22E-03	0.03	0.55	0.42
5	1.65E-04	5.06E-03	1.78E-05	1.29	1.01E-06	2.10E-03	0.03	0.54	0.43
8	1.62E-04	4.97E-03	1.78E-05	1.51	1.05E-06	2.00E-03	0.03	0.52	0.45
7	1.59E-04	4.88E-03	1.78E-05	1.75	1.08E-06	1.92E-03	0.03	0.51	0.46
8	1.56E-04	4.78E-03	1.79E-05	2.01	1.09E-06	1.84E-03	0.03	0.50	0.47

Table S17: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 20 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	9.82E-06	1.88E-04	0.51	0.49	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	1.03E-05	1.77E-04	0.51	0.49	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	1.07E-05	1.69E-04	0.50	0.50	0.00
4	1.68E-04	3.22E-04	1.79E-05	1.10	1.09E-05	1.63E-04	0.49	0.50	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	1.10E-05	1.57E-04	0.47	0.51	0.02
8	1.62E-04	3.22E-04	1.78E-05	1.53	1.11E-05	1.53E-04	0.46	0.51	0.03
7	1.59E-04	3.22E-04	1.78E-05	1.76	1.11E-05	1.50E-04	0.44	0.53	0.03
8	1.56E-04	3.22E-04	1.77E-05	2.01	1.10E-05	1.47E-04	0.43	0.54	0.03

Table S18: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 30 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	9.56E-06	1.85E-04	0.52	0.48	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	1.01E-05	1.74E-04	0.53	0.47	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	1.04E-05	1.66E-04	0.51	0.48	0.01
4	1.68E-04	3.22E-04	1.79E-05	1.10	1.07E-05	1.60E-04	0.50	0.49	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	1.08E-05	1.54E-04	0.49	0.49	0.02
8	1.62E-04	3.22E-04	1.78E-05	1.53	1.09E-05	1.50E-04	0.47	0.50	0.03
7	1.59E-04	3.22E-04	1.78E-05	1.76	1.08E-05	1.47E-04	0.46	0.51	0.03
8	1.56E-04	3.22E-04	1.77E-05	2.01	1.08E-05	1.44E-04	0.44	0.52	0.04

Table S19: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 40 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	9.24E-06	1.81E-04	0.53	0.47	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	9.79E-06	1.70E-04	0.53	0.47	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	1.01E-05	1.62E-04	0.53	0.47	0.00
4	1.68E-04	3.22E-04	1.79E-05	1.10	1.04E-05	1.56E-04	0.51	0.48	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	1.05E-05	1.51E-04	0.51	0.48	0.01
8	1.62E-04	3.22E-04	1.78E-05	1.53	1.06E-05	1.46E-04	0.48	0.49	0.02
7	1.59E-04	3.22E-04	1.78E-05	1.76	1.06E-05	1.43E-04	0.48	0.50	0.02
8	1.56E-04	3.22E-04	1.77E-05	2.01	1.05E-05	1.40E-04	0.45	0.52	0.03

Table S20: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 50 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	8.90E-06	1.77E-04	0.55	0.45	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	9.46E-06	1.66E-04	0.54	0.46	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	9.83E-06	1.58E-04	0.54	0.46	0.00
4	1.68E-04	3.22E-04	1.79E-05	1.10	1.01E-05	1.52E-04	0.53	0.46	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	1.02E-05	1.47E-04	0.52	0.47	0.01
8	1.62E-04	3.22E-04	1.78E-05	1.53	1.03E-05	1.43E-04	0.50	0.47	0.03
7	1.59E-04	3.22E-04	1.78E-05	1.76	1.03E-05	1.40E-04	0.49	0.49	0.02
8	1.56E-04	3.22E-04	1.77E-05	2.01	1.02E-05	1.37E-04	0.47	0.50	0.03

Table S21 sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 60 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	8.52E-06	1.73E-04	0.58	0.42	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	9.10E-06	1.62E-04	0.58	0.42	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	9.47E-06	1.55E-04	0.58	0.42	0.00
4	1.68E-04	3.22E-04	1.79E-05	1.10	9.72E-06	1.48E-04	0.57	0.43	0.00
5	1.65E-04	3.22E-04	1.78E-05	1.31	9.88E-06	1.43E-04	0.56	0.43	0.01
8	1.62E-04	3.22E-04	1.78E-05	1.53	9.95E-06	1.39E-04	0.54	0.44	0.02
7	1.59E-04	3.22E-04	1.78E-05	1.76	9.96E-06	1.36E-04	0.54	0.44	0.02
8	1.56E-04	3.22E-04	1.77E-05	2.01	9.91E-06	1.34E-04	0.53	0.46	0.01

Table S22: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 70 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	8.11E-06	1.69E-04	0.59	0.41	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	8.69E-06	1.58E-04	0.59	0.41	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	9.08E-06	1.50E-04	0.59	0.41	0.00
4	1.68E-04	3.22E-04	1.79E-05	1.10	9.33E-06	1.44E-04	0.59	0.41	0.00
5	1.65E-04	3.22E-04	1.78E-05	1.31	9.50E-06	1.40E-04	0.57	0.42	0.01
8	1.62E-04	3.22E-04	1.78E-05	1.53	9.58E-06	1.36E-04	0.55	0.43	0.02
7	1.59E-04	3.22E-04	1.78E-05	1.76	9.59E-06	1.33E-04	0.55	0.44	0.01
8	1.56E-04	3.22E-04	1.77E-05	2.01	9.54E-06	1.30E-04	0.54	0.45	0.01

Table S23: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 80 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	$(NaClO_4)$	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	7.67E-06	1.65E-04	0.60	0.40	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	8.27E-06	1.55E-04	0.61	0.39	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	8.66E-06	1.47E-04	0.59	0.40	0.01
4	1.68E-04	3.22E-04	1.79E-05	1.10	8.93E-06	1.41E-04	0.59	0.40	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	9.10E-06	1.36E-04	0.59	0.40	0.01
8	1.62E-04	3.22E-04	1.78E-05	1.53	9.18E-06	1.33E-04	0.56	0.42	0.02
7	1.59E-04	3.22E-04	1.78E-05	1.76	9.20E-06	1.30E-04	0.56	0.42	0.02
8	1.56E-04	3.22E-04	1.77E-05	2.01	9.15E-06	1.27E-04	0.54	0.44	0.02

Table S24: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaClO_4)$ at T = 85 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	($NaClO_4$)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.75E-04	3.22E-04	1.79E-05	0.53	7.34E-06	1.59E-04	0.60	0.40	0.00
2	1.73E-04	3.22E-04	1.79E-05	0.71	7.93E-06	1.49E-04	0.60	0.40	0.00
3	1.71E-04	3.22E-04	1.79E-05	0.90	8.33E-06	1.41E-04	0.59	0.40	0.01
4	1.68E-04	3.22E-04	1.79E-05	1.10	8.60E-06	1.35E-04	0.59	0.40	0.01
5	1.65E-04	3.22E-04	1.78E-05	1.31	8.77E-06	1.30E-04	0.58	0.40	0.02
8	1.62E-04	3.22E-04	1.78E-05	1.53	8.86E-06	1.26E-04	0.57	0.40	0.03
7	1.59E-04	3.22E-04	1.78E-05	1.76	8.88E-06	1.23E-04	0.55	0.42	0.03
8	1.56E-04	3.22E-04	1.77E-05	2.01	8.83E-06	1.21E-04	0.55	0.42	0.03

Used background electrolyte: NaCl

Table S25: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaCl)$ at T = 20 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	(NaCl)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	1.32E-06	3.18E-03	0.01	0.49	0.49
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.71E-06	2.76E-03	0.01	0.52	0.47
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.92E-06	2.50E-03	0.01	0.49	0.50
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.99E-06	2.36E-03	0.01	0.50	0.49
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.98E-06	2.26E-03	0.02	0.49	0.49
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.92E-06	2.20E-03	0.02	0.47	0.51
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.82E-06	2.16E-03	0.01	0.45	0.54
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.69E-06	2.14E-03	0.01	0.42	0.57

Table S26: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of $I_m(NaCl)$ at T = 30 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$	(NaCl)	$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	1.34E-06	3.28E-03	0.00	0.52	0.48
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.74E-06	2.89E-03	0.01	0.54	0.45
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.96E-06	2.65E-03	0.01	0.51	0.48
4	1.65E-04	5.28E-03	1.97E-05	1.89	2.03E-06	2.52E-03	0.01	0.52	0.47
5	1.65E-04	5.28E-03	1.97E-05	2.36	2.02E-06	2.43E-03	0.01	0.50	0.49
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.96E-06	2.37E-03	0.01	0.49	0.50
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.86E-06	2.34E-03	0.01	0.47	0.52
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.73E-06	2.32E-03	0.01	0.44	0.55

Table S27: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 40 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	1.24E-06	3.19E-03	0.00	0.58	0.42
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.62E-06	2.80E-03	0.00	0.60	0.40
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.83E-06	2.55E-03	0.01	0.56	0.43
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.90E-06	2.42E-03	0.01	0.58	0.41
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.89E-06	2.33E-03	0.01	0.57	0.42
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.83E-06	2.27E-03	0.01	0.56	0.43
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.74E-06	2.24E-03	0.01	0.54	0.45
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.62E-06	2.22E-03	0.00	0.52	0.48

Table S28: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 50 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	1.13E-06	3.09E-03	0.00	0.56	0.44
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.49E-06	2.69E-03	0.00	0.59	0.41
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.69E-06	2.45E-03	0.00	0.56	0.44
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.76E-06	2.32E-03	0.00	0.58	0.42
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.75E-06	2.23E-03	0.00	0.57	0.43
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.70E-06	2.17E-03	0.00	0.56	0.44
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.62E-06	2.14E-03	0.00	0.55	0.45
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.50E-06	2.12E-03	0.00	0.52	0.48

Table S29: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 60 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	1.02E-06	2.99E-03	0.01	0.59	0.40
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.36E-06	2.59E-03	0.03	0.60	0.37
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.55E-06	2.35E-03	0.03	0.61	0.36
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.61E-06	2.21E-03	0.03	0.60	0.37
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.61E-06	2.13E-03	0.03	0.59	0.37
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.57E-06	2.07E-03	0.03	0.59	0.38
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.49E-06	2.04E-03	0.03	0.57	0.40
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.38E-06	2.02E-03	0.03	0.56	0.41

Table S30: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 70 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	9.20E-07	2.88E-03	0.03	0.60	0.37
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.23E-06	2.48E-03	0.03	0.63	0.34
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.41E-06	2.24E-03	0.03	0.64	0.33
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.47E-06	2.11E-03	0.03	0.63	0.34
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.47E-06	2.02E-03	0.03	0.62	0.34
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.43E-06	1.97E-03	0.03	0.61	0.36
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.36E-06	1.93E-03	0.03	0.61	0.36
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.26E-06	1.91E-03	0.03	0.59	0.38

Table S31: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 80 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	8.19E-07	2.76E-03	0.03	0.62	0.35
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.10E-06	2.36E-03	0.03	0.66	0.31
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.27E-06	2.12E-03	0.03	0.67	0.30
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.33E-06	2.00E-03	0.03	0.66	0.30
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.33E-06	1.91E-03	0.05	0.65	0.29
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.29E-06	1.86E-03	0.05	0.63	0.32
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.23E-06	1.83E-03	0.06	0.63	0.32
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.14E-06	1.81E-03	0.06	0.61	0.33

Table S32: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 85 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	5.28E-03	1.97E-05	0.48	7.70E-07	2.70E-03	0.04	0.62	0.34
2	1.65E-04	5.28E-03	1.97E-05	0.92	1.04E-06	2.30E-03	0.05	0.64	0.31
3	1.65E-04	5.28E-03	1.97E-05	1.42	1.20E-06	2.07E-03	0.05	0.67	0.28
4	1.65E-04	5.28E-03	1.97E-05	1.89	1.26E-06	1.94E-03	0.05	0.66	0.28
5	1.65E-04	5.28E-03	1.97E-05	2.36	1.26E-06	1.86E-03			
8	1.65E-04	5.28E-03	1.97E-05	2.85	1.23E-06	1.81E-03	0.05	0.65	0.29
7	1.65E-04	5.28E-03	1.97E-05	3.34	1.17E-06	1.77E-03	0.06	0.64	0.30
8	1.65E-04	5.28E-03	1.97E-05	3.87	1.09E-06	1.76E-03	0.06	0.63	0.31

Table S33: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 20 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.40E-05	9.29E-05	0.70	0.30	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.51E-05	7.97E-05	0.75	0.25	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.55E-05	7.31E-05	0.74	0.26	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.56E-05	6.88E-05	0.74	0.26	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.56E-05	6.60E-05	0.74	0.26	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.55E-05	6.43E-05	0.75	0.25	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.53E-05	6.33E-05			
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.50E-05	6.26E-05	0.76	0.24	0.00

Table S34: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 30 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.41E-05	9.61E-05	0.72	0.28	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.52E-05	8.38E-05	0.76	0.24	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.56E-05	7.76E-05	0.76	0.24	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.57E-05	7.36E-05	0.75	0.25	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.57E-05	7.10E-05	0.75	0.25	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.55E-05	6.94E-05	0.76	0.24	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.54E-05	6.84E-05	0.75	0.25	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.51E-05	6.78E-05	0.76	0.24	0.00

Table S35: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 40 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.37E-05	9.32E-05	0.74	0.26	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.49E-05	8.08E-05	0.78	0.22	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.53E-05	7.46E-05	0.78	0.22	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.55E-05	7.06E-05	0.77	0.23	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.54E-05	6.80E-05	0.77	0.23	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.53E-05	6.65E-05	0.77	0.23	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.51E-05	6.55E-05	0.76	0.24	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.48E-05	6.49E-05	0.76	0.24	0.00

Table S36: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 50 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.33E-05	9.01E-05	0.76	0.24	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.46E-05	7.77E-05	0.79	0.21	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.50E-05	7.15E-05	0.78	0.22	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.52E-05	6.75E-05	0.78	0.22	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.52E-05	6.50E-05	0.77	0.23	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.50E-05	6.34E-05	0.78	0.22	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.48E-05	6.25E-05	0.77	0.23	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.45E-05	6.19E-05	0.77	0.23	0.00

Table S37: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 60 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.29E-05	8.68E-05	0.78	0.22	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.42E-05	7.44E-05	0.81	0.19	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.47E-05	6.83E-05	0.81	0.19	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.49E-05	6.43E-05	0.79	0.21	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.48E-05	6.18E-05	0.79	0.21	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.47E-05	6.03E-05	0.79	0.21	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.45E-05	5.94E-05	0.78	0.22	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.42E-05	5.88E-05	0.78	0.22	0.00

Table S38: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 70 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.24E-05	8.34E-05	0.80	0.20	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.38E-05	7.09E-05	0.82	0.18	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.43E-05	6.49E-05	0.82	0.18	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.45E-05	6.10E-05	0.81	0.19	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.45E-05	5.86E-05	0.80	0.20	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.43E-05	5.71E-05	0.80	0.20	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.41E-05	5.62E-05	0.80	0.20	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.38E-05	5.56E-05	0.80	0.20	0.00

Table S39: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 80 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.18E-05	7.98E-05	0.84	0.16	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.34E-05	6.74E-05	0.85	0.15	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.39E-05	6.15E-05	0.84	0.16	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.41E-05	5.77E-05	0.82	0.18	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.41E-05	5.53E-05	0.81	0.19	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.39E-05	5.38E-05	0.80	0.20	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.37E-05	5.29E-05	0.80	0.20	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.34E-05	5.24E-05	0.80	0.20	0.00

Table S40: sample composition for the determination of ionic strength effects for the complexation of Np(V) with Ox^{2-} as a function of I_m(NaCl) at T = 85 °C and species distribution obtained by principle component analyses of the absorption spectra.

Nr.	total concentrations			I_m (NaCl)	eq. concentration		species fractions χ_i		
	$[NpO_2^+]_{total}$	$[Ox^{2-}]_{total}$	$[H^+]_{total}$		$[H^+]_{eq}$	$[Ox^{2-}]_{eq}$	NpO_2^+	$NpO_2(Ox)^-$	$NpO_2(Ox)_2^{3-}$
1	1.65E-04	1.59E-04	1.97E-05	0.47	1.15E-05	7.79E-05	0.86	0.14	0.00
2	1.65E-04	1.59E-04	1.97E-05	0.98	1.31E-05	6.56E-05	0.86	0.14	0.00
3	1.65E-04	1.59E-04	1.97E-05	1.46	1.37E-05	5.97E-05	0.84	0.16	0.00
4	1.65E-04	1.59E-04	1.97E-05	1.96	1.38E-05	5.60E-05	0.82	0.18	0.00
5	1.65E-04	1.59E-04	1.97E-05	2.48	1.38E-05	5.36E-05	0.81	0.19	0.00
8	1.65E-04	1.59E-04	1.97E-05	2.96	1.37E-05	5.22E-05	0.81	0.19	0.00
7	1.65E-04	1.59E-04	1.97E-05	3.43	1.35E-05	5.13E-05	0.81	0.19	0.00
8	1.65E-04	1.59E-04	1.97E-05	3.93	1.31E-05	5.08E-05	0.81	0.19	0.00