Precipitation of morphology-controlled uranium(VI) peroxide in nitric acid media

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Table SI 1 : Initials conditions for all precipitations.

ID	$C(U)_{ini}$ ($mol \cdot L^{-1}$)	$C(H^+)_{ini}$ ($mol \cdot L^{-1}$)	$C(NO_3^-)_{ini}$ ($mol \cdot L^{-1}$)	$C(H_2O_2)_{ini}/C(U)_{ini}$	SI_{ini}	Time (min)	Final yield (%)	Final reaction progress (%)	U measuring method
1	0.068 ± 0.001	0.1	0.24	10	3.5	293	99.9 ± 0.3	99.9 ± 0.3	ICP-OES
2	0.069 ± 0.001	0.1	0.24	20	3.8	60	99.8 ± 0.3	99.8 ± 0.3	PERALS
3	0.068 ± 0.001	0.1	0.24	68	4.3	60	98.2 ± 0.4	98.2 ± 0.4	PERALS
4	0.067 ± 0.001	0.5	0.63	1	1.1	150	20.8 ± 11.7	26.5 ± 11.7	PERALS
5	0.068 ± 0.001	0.5	0.64	5	1.8	60	58.7 ± 6.0	59.2 ± 6.0	PERALS
6	0.068 ± 0.001	0.5	0.64	10	2.1	500	90.2 ± 1.5	90.5 ± 1.5	PERALS
7	0.068 ± 0.001	0.5	0.64	10	2.1	60	97.7 ± 0.5	98.1 ± 0.5	ICP-OES
8	0.070 ± 0.001	0.5	0.64	10	2.1	128	91.5 ± 1.2	91.8 ± 1.2	PERALS
9	0.068 ± 0.001	0.5	0.64	20	2.4	131	98.7 ± 0.3	98.9 ± 0.3	ICP-OES
10	0.067 ± 0.001	0.5	0.63	20	2.4	189	98.2 ± 0.4	98.4 ± 0.4	ICP-OES
11	0.067 ± 0.001	0.5	0.63	30	2.6	129	98.7 ± 0.4	98.9 ± 0.4	PERALS
12	0.068 ± 0.001	0.5	0.64	60	2.9	60	99.3 ± 0.3	99.4 ± 0.3	PERALS
13	0.069 ± 0.001	0.5	0.64	68	3.0	60	94.6 ± 0.8	94.7 ± 0.8	ICP-OES
14	0.070 ± 0.001	1.0	1.14	5	1.2	380	26.8 ± 10.5	28.2 ± 10.5	ICP-OES
15	0.074 ± 0.001	1.0	1.15	10	1.5	501	93.3 ± 0.9	95.3 ± 0.9	PERALS
16	0.069 ± 0.001	1.0	1.14	15	1.7	434	96.3 ± 0.6	97.7 ± 0.6	PERALS
17	0.068 ± 0.001	1.0	1.14	20	1.8	60	88.5 ± 1.7	89.5 ± 1.7	ICP-OES
18	0.067 ± 0.001	1.0	1.14	20	1.8	236	99.1 ± 0.3	100.3 ± 0.3	ICP-OES
19	0.068 ± 0.001	1.0	1.14	40	2.1	243	97.9 ± 0.4	98.5 ± 0.4	PERALS
20	0.066 ± 0.001	1.0	1.14	68	2.3	60	87.5 ± 1.9	87.8 ± 1.9	ICP-OES
21	0.070 ± 0.001	2.0	2.14	10	0.9	501	58.6 ± 5.9	65.5 ± 5.9	PERALS
22	0.069 ± 0.001	2.0	2.14	20	1.2	60	23.9 ± 11.0	25.2 ± 11.0	ICP-OES
23	0.068 ± 0.001	2.0	2.14	20	1.2	208	95.3 ± 0.8	100.6 ± 0.8	PERALS
24	0.069 ± 0.001	2.0	2.14	60	1.7	434	99.2 ± 0.3	100.9 ± 0.3	PERALS
25	0.071 ± 0.001	2.0	2.14	68	1.7	60	49.7 ± 7.1	50.4 ± 7.1	PERALS

Table SI 2 : Lattice parameter, crystallite size for each refinement and weighted profile R-factor (Rwp) of the refinement of each sample.

ID	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Cell volume (Å^3)	Crystallite size (nm)	Rwp
1	14.221 ± 0.014	6.774 ± 0.014	8.505 ± 0.017	123.409 ± 0.062	683.92 ± 0.08	37 ± 6	16.0
2	14.235 ± 0.014	6.752 ± 0.014	8.510 ± 0.017	123.406 ± 0.062	682.85 ± 0.08	25 ± 4	16.3
3	14.205 ± 0.014	6.782 ± 0.014	8.504 ± 0.017	123.374 ± 0.062	684.19 ± 0.08	18 ± 3	15.3
4	14.149 ± 0.014	6.778 ± 0.014	8.495 ± 0.017	123.248 ± 0.062	681.38 ± 0.08	81 ± 12	18.8
5	14.165 ± 0.014	6.775 ± 0.014	8.503 ± 0.017	123.312 ± 0.062	681.95 ± 0.08	42 ± 6	28.4
6	14.179 ± 0.014	6.771 ± 0.014	8.498 ± 0.017	123.381 ± 0.062	681.24 ± 0.08	68 ± 10	15.4
7	14.166 ± 0.014	6.770 ± 0.014	8.498 ± 0.017	123.334 ± 0.062	680.96 ± 0.08	82 ± 12	13.4
8	14.166 ± 0.014	6.771 ± 0.014	8.496 ± 0.017	123.345 ± 0.062	680.76 ± 0.08	74 ± 11	11.3
9	14.211 ± 0.014	6.764 ± 0.014	8.508 ± 0.017	123.433 ± 0.062	682.48 ± 0.08	53 ± 8	12.5
10	14.180 ± 0.014	6.762 ± 0.014	8.496 ± 0.017	123.457 ± 0.062	679.71 ± 0.08	46 ± 7	15.7
11	14.196 ± 0.014	6.765 ± 0.014	8.498 ± 0.017	123.471 ± 0.062	680.75 ± 0.08	41 ± 6	15.7
12	14.224 ± 0.014	6.759 ± 0.014	8.498 ± 0.017	123.534 ± 0.062	680.99 ± 0.08	35 ± 5	15.9
13	14.250 ± 0.014	6.765 ± 0.014	8.507 ± 0.017	123.583 ± 0.062	683.27 ± 0.08	26 ± 4	15.4
14	14.165 ± 0.014	6.777 ± 0.014	8.499 ± 0.017	123.203 ± 0.062	682.61 ± 0.08	144 ± 22	15.9
15	14.153 ± 0.014	6.773 ± 0.014	8.494 ± 0.017	123.273 ± 0.062	680.68 ± 0.08	109 ± 16	12.3
16	14.159 ± 0.014	6.773 ± 0.014	8.494 ± 0.017	123.344 ± 0.062	680.47 ± 0.08	44 ± 7	12.6
17	14.170 ± 0.014	6.770 ± 0.014	8.499 ± 0.017	123.333 ± 0.062	681.23 ± 0.08	73 ± 11	16.0
18	14.168 ± 0.014	6.774 ± 0.014	8.499 ± 0.017	123.331 ± 0.062	681.52 ± 0.08	52 ± 8	18.4
19	14.175 ± 0.014	6.765 ± 0.014	8.493 ± 0.017	123.396 ± 0.062	679.95 ± 0.08	113 ± 17	13.1
20	14.191 ± 0.014	6.763 ± 0.014	8.496 ± 0.017	123.429 ± 0.062	680.48 ± 0.08	95 ± 14	16.2
21	14.151 ± 0.014	6.773 ± 0.014	8.495 ± 0.017	123.250 ± 0.062	680.90 ± 0.08	180 ± 27	11.6
22	14.167 ± 0.014	6.773 ± 0.014	8.482 ± 0.017	123.264 ± 0.062	680.54 ± 0.08	114 ± 17	18.4
24	14.153 ± 0.014	6.770 ± 0.014	8.482 ± 0.017	123.311 ± 0.062	679.17 ± 0.08	54 ± 8	15.6
25	14.168 ± 0.014	6.774 ± 0.014	8.491 ± 0.017	123.310 ± 0.062	681.01 ± 0.08	182 ± 27	14.4

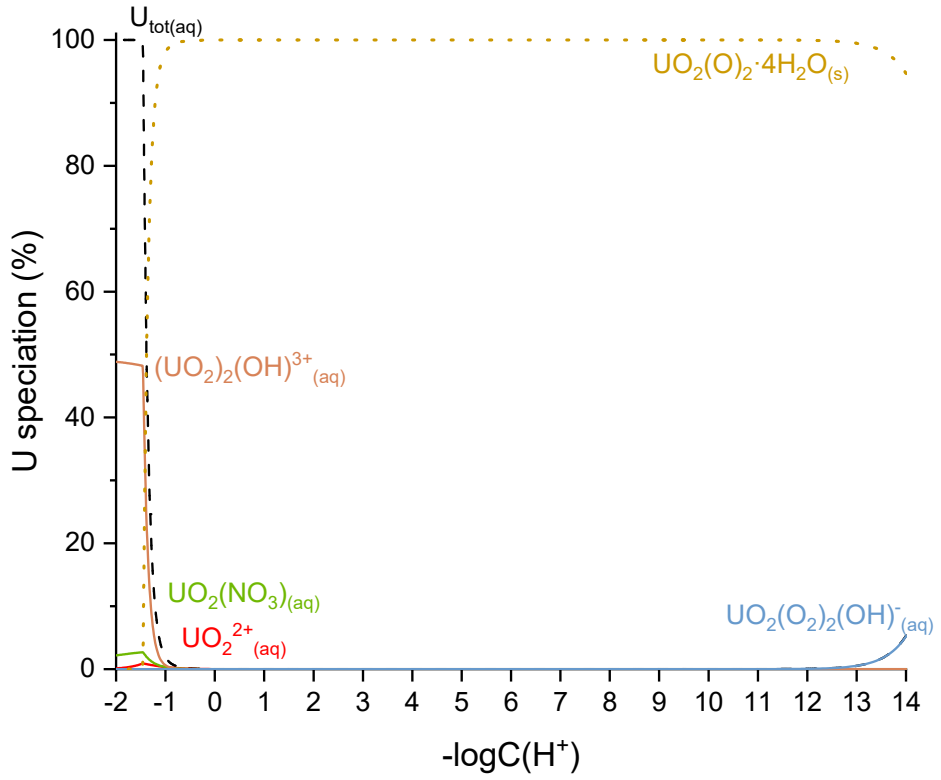

Fig SI 1 : Speciation of the U(VI)-H_2O_2-HNO_3 System as a Function of Acidity ; $C(U)_{tot}$ = 0.068 mol·L^{-1}, $C(NO_3^-)$ = 0.135 mol·L^{-1} ; $C(H_2O_2)$ = 4.634 mol·L^{-1} ($C(H_2O_2)/C(U)$ = 68).

Table SI 3 : Reaction formation and thermodynamic constants of species added in Phreeqc simulations.

Reactions	**$\log_{10}K^0$**	**Reference**
$H_2O_2 \rightleftharpoons HO_2^- + H^+$	– 11.62	[1]
$UO_2^{2+} + H_2O + HO_2^- \rightleftharpoons [(UO_2)(O_2)(OH)]^- + 2\ H^+$	– 2.340 ± 0.070	[2]
$2\ UO_2^{2+} + H_2O + 2\ HO_2^- \rightleftharpoons [(UO_2)_2(O_2)_2(OH)]^- + 3\ H^+$	7.99 ± 0.160	[2]

References

[1] Lide, D. R. *CRC Handbook of Chemistry and Physics, 85th Edition*; CRC Press, *2004*.

[2] OECD. *Second update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium And Technetium, Volume 14*; Organisation for Economic Co-operation and Development: Paris, *2021*.