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Supplement for the article:

Synthesis, characterization and thermodynamics of arsenates forming in the Ca-Fe(III)-As(V)-NO₃ system: Implications for the stability of Ca-Fe arsenates

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5 Pages (including cover page)

4 Figures

2 Tables

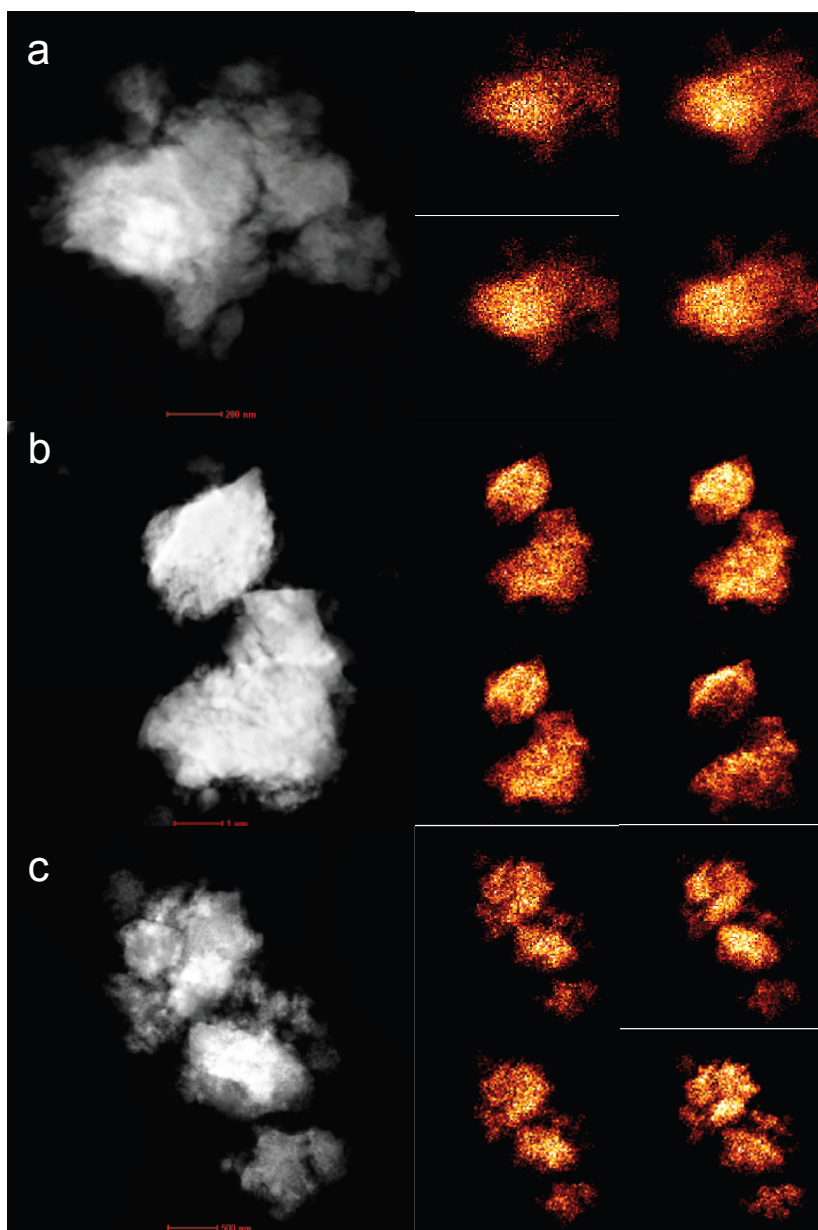


Figure S1. Scanning transmission electron microscopy (STEM) images of precipitates (left) formed at pH 6 after 13 h (a), at pH 7 after 13 h (b) and at pH 9 after 24 h (c). Precipitates are agglomerations of nanoparticles. Corresponding X-ray maps of Ca and Fe (upper row) and As and O maps (lower row). Widths of STEM images are 1.4, 7.6 and 4.25 μm .

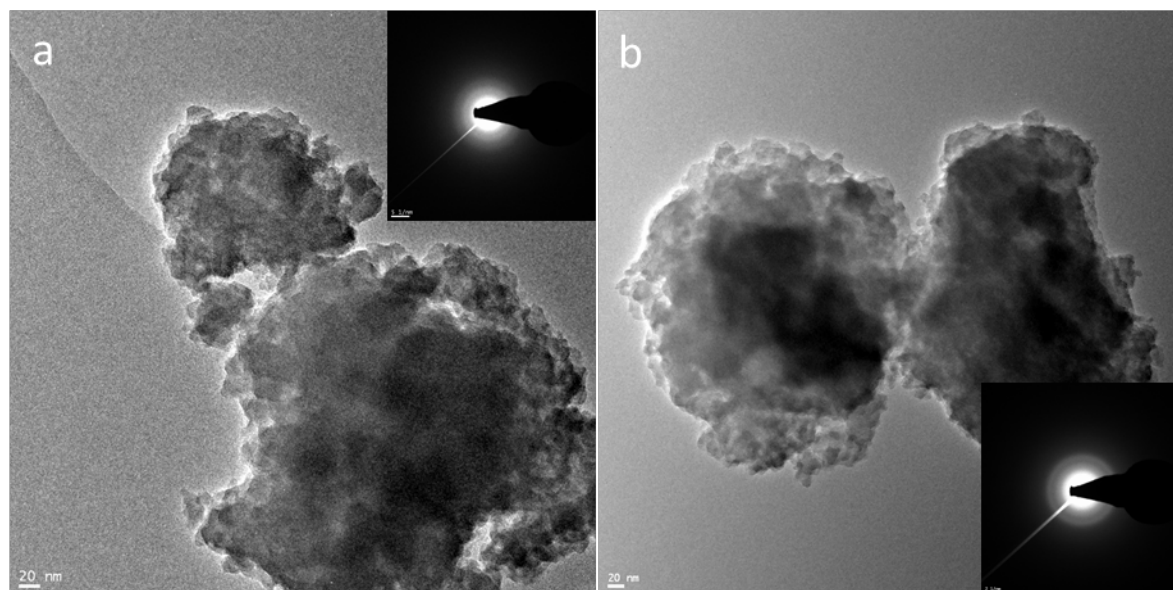


Figure S2. TEM photomicrographs of initial Ca-Fe arsenate precipitates and their selected area diffraction patterns (inset). Scale bars for photomicrographs are 20 nm. (a) precipitate formed at pH 6 at 1 h (K09); (b) precipitate formed at pH 11 at 1 h (K11).

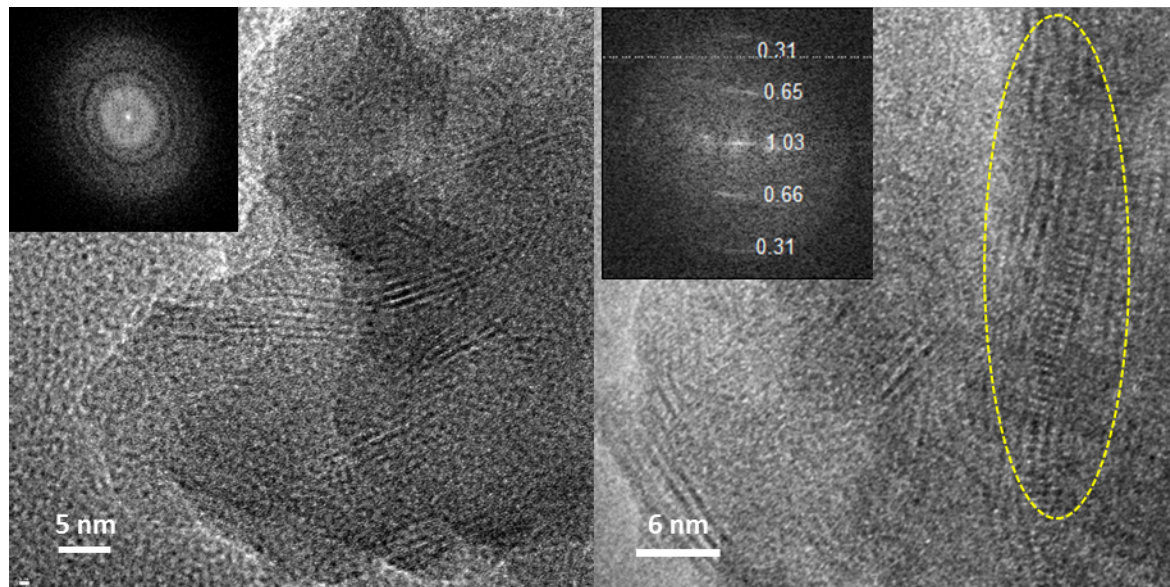


Figure S3. HRTEM photomicrographs of intermediary precipitates formed at pH 6 after 24 h (K09). (a) lattice fringe spacings obtained through Fast Fourier Transform of image (a) are 0.32, 0.36, 0.42, 0.56 and 0.99 nm (inset), and the area outlined by yellow ellipsoid in image (b) are 0.31, 0.65 and 1.03 nm (inset).

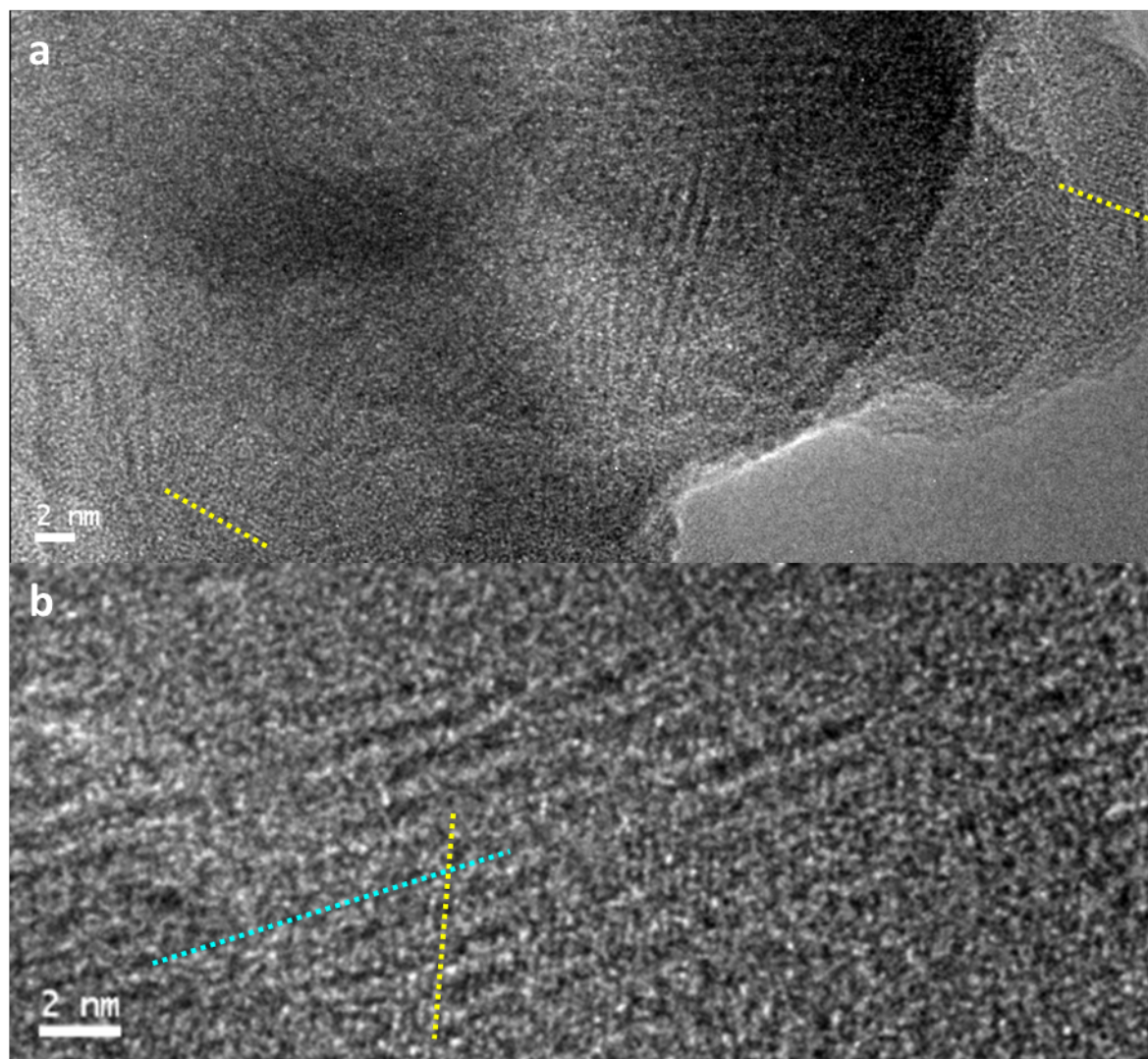


Figure S4. HRTEM images showing lattice fringes highlighted by yellow dotted lines in (a) have 0.27-0.29 nm spacings. Lattice fringes highlighted by cyan dotted line have spacings of 0.98 nm and represent (100) octahedral layers, and those highlighted by yellow dotted lines have spacings of 0.27 nm.

Table S1. Chemical compositions of the precipitates based on semi-quantitative microanalysis under TEM

	K09-1	K09-24	K11-1	K11-24	Nominal
wt%	cfa	yuk	cfa	yuk	yuk
Fe	28.9	25.9	25.5	32.6	
Ca	8.5	8.6	12.3	11.4	
As	34.0	33.1	29.9	33.2	
<i>formula</i>					
Fe	3.0	3.0	3.0	3.0	3.0
Ca	1.2	1.4	2.0	1.5	1.4
AsO ₄	2.6	2.9	2.6	2.3	2.1

Mineral formula based on 17 O recast to 3 Fe. Nominal based on yukonite from Daulton Mine, Yukon (Table 1).

Table S2. Thermodynamic functions for arseniosiderite

T K	C_p $J\ mol^{-1}\ K^{-1}$	H_T-H_0 $kJ\ mol^{-1}$	S $J\ mol^{-1}\ K^{-1}$	G_T-G_0 $kJ\ mol^{-1}$
0	0	0	0*	0
5	0.4544	0.7885	0.2299	-0.3609
10	1.917	6.202	0.9225	-3.023
15	4.236	21.10	2.097	-10.36
20	7.498	50.59	3.766	-24.73
25	11.51	98.07	5.866	-48.58
30	16.00	168.4	8.420	-84.18
35	21.27	261.2	11.27	-133.2
40	26.97	381.6	14.47	-197.3
45	33.30	531.8	18.00	-278.2
50	38.84	710.7	21.76	-377.3
55	44.91	920.8	25.76	-495.9
60	51.29	1162	29.95	-635.1
65	57.45	1433	34.29	-795.6
70	63.43	1736	38.77	-978.1
75	69.30	2067	43.34	-1183
80	76.23	2432	48.04	-1412
85	80.22	2823	52.79	-1664
90	87.35	3245	57.6	-1940
95	91.84	3693	62.45	-2240
100	97.95	4170	67.34	-2564
110	108.7	5195	77.10	-3286
120	121.7	6347	87.11	-4106
130	129.8	7608	97.20	-5028
140	137.0	8942	107.1	-6050
150	144.0	10350	116.8	-7170
160	149.8	11820	126.3	-8386
170	154.3	13340	135.5	-9696
180	159.1	14910	144.5	-11100
190	164.6	16530	153.2	-12580
200	169.7	18200	161.8	-14160
210	174.1	19920	170.2	-15820
220	178.2	21680	178.4	-17560
230	182.5	23480	186.4	-19390
240	187.1	25330	194.2	-21290
250	191.1	27220	202.0	-23270
260	195.5	29150	209.5	-25330
270	199.7	31130	217.0	-27460
273.15	200.9	31760	219.3	-28150
280	203.5	33140	224.3	-29670
290	209.0	35210	231.6	-31950
298.15	212.8	36930	237.4	-33860
300	213.6	37320	238.7	-34300

*Nominal value (see text).